Large Scale Shell-Model Calculations for Open-shell nuclei

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Large Scale Shell-Model Calculations for Open-shell nuclei

Part I: The BIGSTICK shell model code

+ W. Erich Ormand (LLNL), Ken McElvain (UC Berkeley), Hongzhang Shan (LBL)

Part II: Applications

II a: Transitions and the Brink-Axel hypothesis

+ Michael K. G. Kruse (LLNL), W. Erich Ormand (LLNL) and Micah Schuster (SDSU)

II b: *ab initio* Gamow-Teller transitions (in progress)

II c: L-S decomposition of *ab initio* nuclides

EXECUTIVE SUMMARY ON THE BIGSTICK CODE

Many-fermion code: 2^{nd} generation after REDSTICK code
(started in *Baton Rouge, La.*)

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 300M+ on desktop
--has done *dimension 9 billion*+ on supercomputers

Inline calculations of one-body density matrices,
single-particle occupations,
(+ options to compute strength functions via Lanczos trick, etc.)
Will add 2-body non-scalar transition operators later this year

45 kilolines of code Fortran 90 + MPI + OpenMP
Plan to release beta version later this year…followed by CPC pub

The Basic Problem

The matrix formalism:

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

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

$$\sum_{\beta} H_{\alpha\beta}c_{\beta} = Ec_{\alpha} \quad \text{if} \qquad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}$$

The Basic Problem

Find extremal eigenvalues of very large, very sparse Hermitian matrix

→ Lanczos algorithm

fundamental operation is *matrix-vector multiply*

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

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

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

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

matrix-vector multiply

Lanczos algorithm!

A Sparse Matrix, but....

Despite sparsity, nonzero matrix elements can require TB of storage

How the basis states are represented

Product wavefunction ("Slater Determinant")

$$\Psi(\vec{r}_1, \vec{r}_2, \vec{r}_3 \ldots) = \phi_{n_1}(\vec{r}_1)\phi_{n_2}(\vec{r}_2)\phi_{n_3}(\vec{r}_3)\ldots\phi_{n_N}(\vec{r}_N)$$

Each many-body state can be *uniquely* determined by a list of "occupied" single-particle states = "occupation representation"

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

A Sparse Matrix, but….

Despite sparsity, nonzero matrix elements can require TB of storage

- Typical dimensions and sparsity

Nuclide	valence space	valence Z	valence N	basis dim	sparsity (%)	
^{20}Ne	"sd"	2	2	640	10	
^{25}Mg	"sd"	4	5	44,133	0.5	
^{49}Cr	"pf"	4	5	6M	0.01	
^{56}Fe	"pf"	6	10	500M	$2x10^{-4}$	
^{12}C	N_{max}=8	6	6	600M	$4x10^{-4}$	2-body force
^{12}C	N_{max}=8	6	6	600M	$2x10^{-2}$	3-body force

A SPARSE MATRIX, BUT….

Despite sparsity, nonzero matrix elements can require TB of storage

Nuclide	Space	Basis dim	matrix store
^{56}Fe	*pf*	501 M	4.2 Tb
^{7}Li	N_{max}=12	252 M	3.6 Tb
^{7}Li	N_{max}=14	1200 M	23 Tb
^{12}C	N_{max}=6	32M	0.2 Tb
^{12}C	N_{max}=8	590M	5 Tb
^{12}C	N_{max}=10	7800M	111 Tb
^{16}O	N_{max}=6	26 M	0.14 Tb
^{16}O	N_{max}=8	990 M	9.7 Tb

Recycled Matrix Elements

Only a fraction of matrix elements are unique; **most are reused.**
Reuse of matrix elements understood through *spectator* particles.

# of nonzero matrix elements vs. # unique matrix elements

Nuclide	valence space	valence Z	valence N	# nonzero	# unique
^{28}Si	"sd"	6	6	26 x 10^6	3600
^{52}Fe	"pf"	6	6	90 x 10^9	21,500

This suggests one can reduce storage of matrix elements…

Factorization

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

A quantum number is the eigenvalue of an operator

generally a operator that exactly commutes with the Hamiltonian

e.g. angular momentum $\mathbf{J}^2$ and *z*-component $\mathbf{J}_z$

$$\hat{J}^2|\Psi\rangle = J(J+1)|\Psi\rangle \qquad \hat{J}_z|\Psi\rangle = M|\Psi\rangle$$

FACTORIZATION

Reuse can be **exploited using exact factorization** enforced through *Abelian* (additive/multiplicative) *quantum numbers*

A quantum number is the eigenvalue of an operator

For composite systems, one can apply the operator to each component separately:

$$\hat{O}|\Psi\rangle = \left(\hat{O}_1 + \hat{O}_2 + \hat{O}_3 + \ldots\right)\left(|\Psi_1\rangle \otimes |\Psi_2\rangle \otimes |\Psi_3\rangle \otimes \ldots\right)$$

Sometimes the total quantum number is a simple sum/product as is the case for $\mathbf{J}_z$ or parity....

$$\hat{J}_z|\Psi\rangle = M|\Psi\rangle = (m_1 + m_2 + m_3 + \ldots)|\Psi\rangle$$

…but in other cases the addition is complicated (e.g. for $\mathbf{J}^2$)

FACTORIZATION

Reuse can be **exploited using exact factorization**
enforced through *additive/multiplicative quantum numbers*

I consider composite many-fermion systems,
in particular those with 2 major components
protons and *neutrons*
or
spin-up and *spin-down* electrons

$$\left|\Psi\right\rangle = \left|\Psi_1\right\rangle \otimes \left|\Psi_2\right\rangle$$

Each component itself is a Slater determinant which is composed of many particles

$$\hat{J}_z\left|\Psi\right\rangle = M\left|\Psi\right\rangle \qquad M = M_1 + M_2$$

$$M_1 = m_1^{(1)} + m_1^{(2)} + m_1^{(2)} + \ldots$$

Factorization

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

Because the M values are discrete integers or half-integers (-3, -2, -1, 0, 1, 2, ... or -3/2, -1/2, +1/2, +3/2....) we can organize the basis states in discrete *sectors*

Example: 2 protons, 4 neutrons, total M = 0

$M_z(\pi) = -4$	$M_z(\upsilon) = +4$
$M_z(\pi) = -3$	$M_z(\upsilon) = +3$
$M_z(\pi) = -2$	$M_z(\upsilon) = +2$

FACTORIZATION

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

In fact, we can see an example of factorization here because all proton Slater determinants in one M-sector *must* combine with all the conjugate neutron Slater determinants

Example: 2 protons, 4 neutrons, total M = 0

$M_z(\pi) = -4$: 2 SDs	$M_z(\upsilon) = +4$: 24 SDs	48 combined
$M_z(\pi) = -3$: 4 SDs	$M_z(\upsilon) = +3$: 39 SDs	156 combined
$M_z(\pi) = -2$: 9 SDs	$M_z(\upsilon) = +2$: 60 SDs	540 combined

Factorization

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

In fact, we can see an example of factorization here because all proton Slater determinants in one M-sector *must* combine with all the conjugate neutron Slater determinants

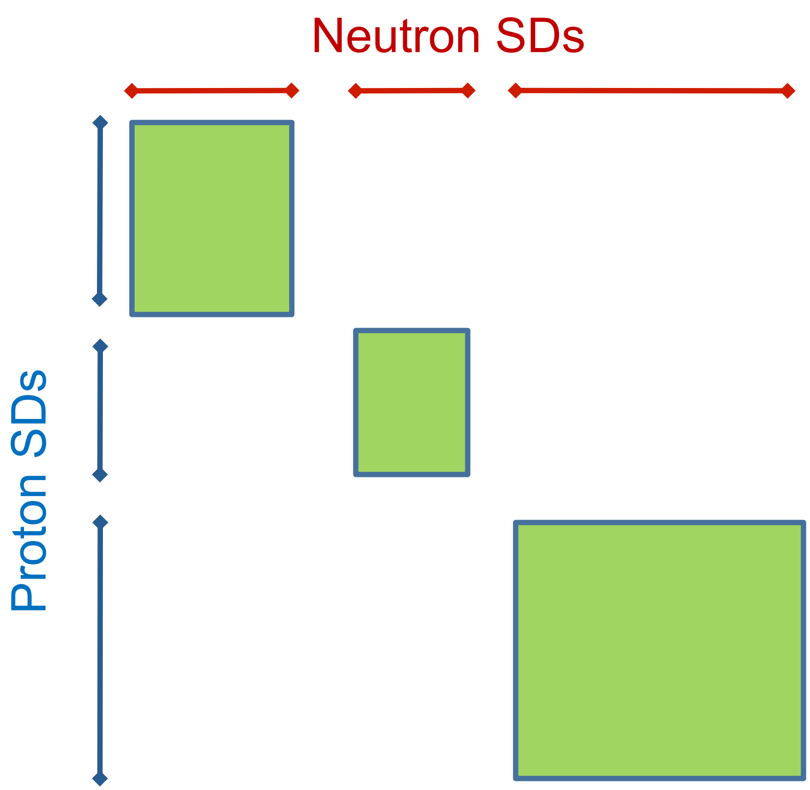
$M_z(\pi)$ = -4: 2 SDs	$M_z(\upsilon)$ = +4: 24 SDs	48 combined

$$
\begin{matrix} |\pi_1\rangle \\ |\pi_2\rangle \end{matrix}
\times
\begin{matrix} |\nu_1\rangle \\ |\nu_2\rangle \\ |\nu_3\rangle \\ |\nu_4\rangle \\ \vdots \\ |\nu_{24}\rangle \end{matrix}
=
\begin{matrix} |\pi_1\rangle|\nu_1\rangle \\ |\pi_2\rangle|\nu_1\rangle \\ |\pi_1\rangle|\nu_2\rangle \\ |\pi_2\rangle|\nu_2\rangle \\ \vdots \\ |\pi_1\rangle|\nu_{24}\rangle \\ |\pi_2\rangle|\nu_{24}\rangle \end{matrix}
$$

FACTORIZATION

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

$$|\alpha\rangle = |\alpha_p\rangle \times |\alpha_n\rangle$$



Example N = Z nuclei

Nuclide	Basis dim	# pSDs (=#nSDs)
^{20}Ne	640	66
^{24}Mg	28,503	495
^{28}Si	93,710	924
^{48}Cr	1,963,461	4895
^{52}Fe	109,954,620	38,760
^{56}Ni	1,087,455,228	125,970

FACTORIZATION

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

Factorization allows us to keep track of all basis states without writing out every one explicitly
-- we only need to write down the proton/neutron components

The same trick can be applied to matrix-vector multiply

$$\hat{H} = \hat{H}_{pp} + \hat{H}_{nn} + \hat{H}_{pn}$$

Move 2 protons; *neutrons are spectators*

Move 2 neutrons; *protons are spectators*

Move 1 proton + 1 neutron; *rest are spectators*

FACTORIZATION

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

$$\hat{H}_{pp}$$

Move 2 protons; *neutrons are spectators*

Example: 2 protons, 4 neutrons, total M = 0

$M_z(\pi) = -4$: 2 SDs	$M_z(\upsilon) = +4$: 24 SDs	48 combined

There are potentially 48 × 48 matrix elements
But for H_{pp} at most 4 × 24 are nonzero
and we only have to look up 4 matrix elements

Advantage: **we can store 98 matrix elements as 4 matrix elements** and avoid 2000+ zero matrix elements.

FACTORIZATION

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

$M_z(\pi)$ = -4: 2 SDs	$M_z(\upsilon)$ = +4: 24 SDs	48 combined

$$|\pi_1\rangle \quad |\pi_2\rangle$$

$$H_{pp} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}$$

$$|\nu_1\rangle \quad |\nu_2\rangle \quad |\nu_3\rangle \quad |\nu_4\rangle \quad \vdots \quad |\nu_{24}\rangle$$

$$H_{pp}|\pi_1\rangle|\nu_1\rangle = H_{11}|\pi_1\rangle|\nu_1\rangle + H_{12}|\pi_2\rangle|\nu_1\rangle$$
$$H_{pp}|\pi_2\rangle|\nu_1\rangle = H_{12}|\pi_1\rangle|\nu_1\rangle + H_{22}|\pi_2\rangle|\nu_1\rangle$$
$$H_{pp}|\pi_1\rangle|\nu_2\rangle = H_{11}|\pi_1\rangle|\nu_2\rangle + H_{12}|\pi_2\rangle|\nu_2\rangle$$
$$H_{pp}|\pi_2\rangle|\nu_2\rangle = H_{12}|\pi_1\rangle|\nu_2\rangle + H_{22}|\pi_2\rangle|\nu_2\rangle$$
$$\vdots$$
$$H_{pp}|\pi_1\rangle|\nu_{24}\rangle = H_{11}|\pi_1\rangle|\nu_{24}\rangle + H_{12}|\pi_2\rangle|\nu_{24}\rangle$$
$$H_{pp}|\pi_2\rangle|\nu_{24}\rangle = H_{12}|\pi_1\rangle|\nu_{24}\rangle + H_{22}|\pi_2\rangle|\nu_{24}\rangle$$

Advantage: **we can store 98 matrix elements as 4 matrix elements** and avoid 2000+ zero matrix elements.

FACTORIZATION

Reuse can be **exploited using exact factorization** enforced through *additive/multiplicative quantum numbers*

Comparison of nonzero matrix storage with factorization

Nuclide	Space	Basis dim	matrix store	factorization
^{56}Fe	*pf*	501 M	290 Gb	0.72 Gb
^{7}Li	N_{max}=12	252 M	3600 Gb	96 Gb
^{7}Li	N_{max}=14	1200 M	23 Tb	624 Gb
^{12}C	N_{max}=6	32M	196 Gb	3.3 Gb
^{12}C	N_{max}=8	590M	5000 Gb	65 Gb
^{12}C	N_{max}=10	7800M	111 Tb	1.4 Tb
^{16}O	N_{max}=6	26 M	142 Gb	3.0 Gb
^{16}O	N_{max}=8	990 M	9700 Gb	130 Gb

Comparison of nonzero matrix storage with factorization

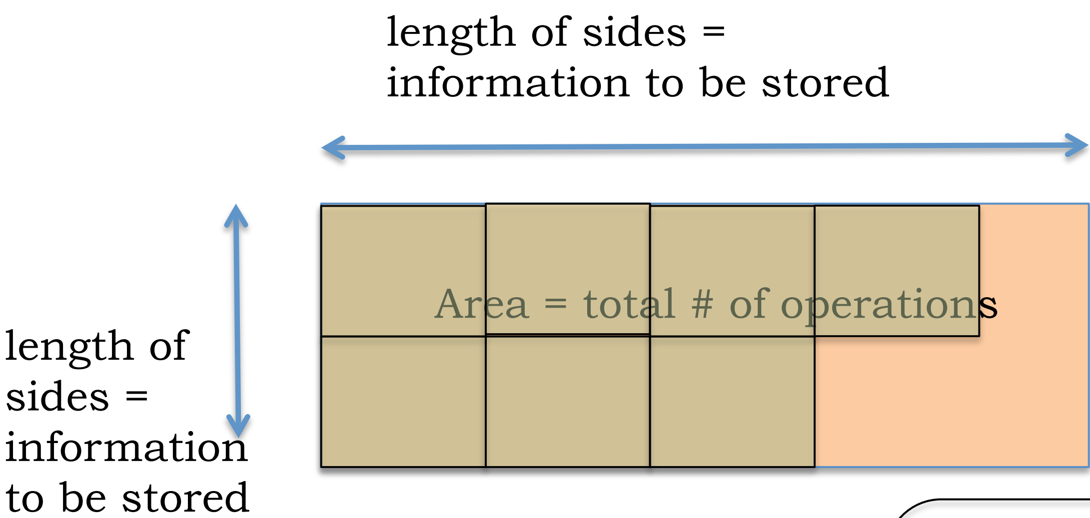
^{7}Li

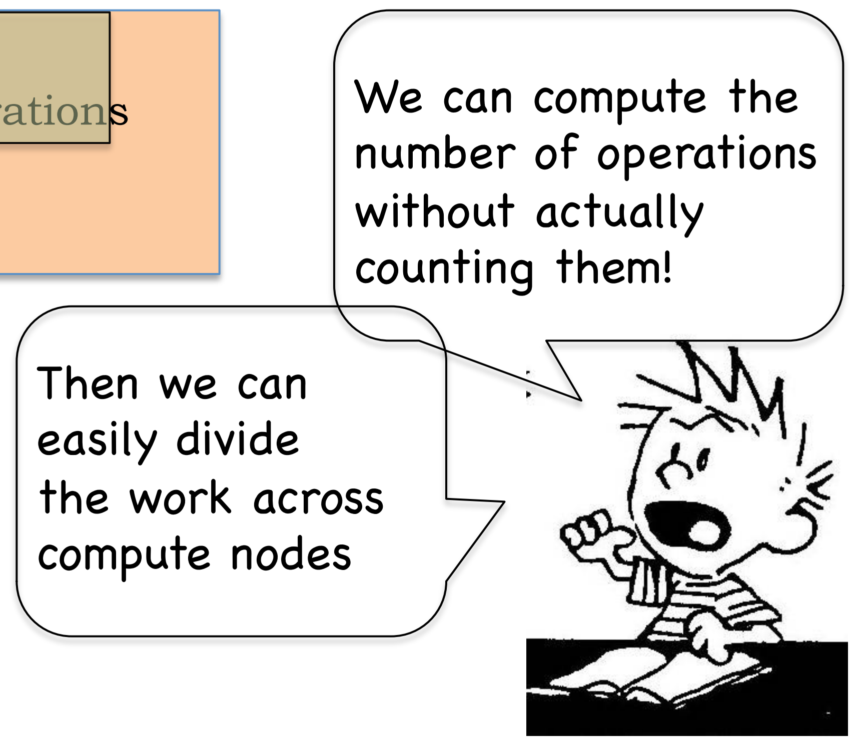
Space	Basis dim	matrix store (2-body)	factorization (2-body)	matrix store (3-body)	factorization (3-body)
$N_{max}=8$	6 M	36 Gb	1.5 Gb	1 Tb	26 Gb
$N_{max}=10$	43 M	430 Gb	10 Gb	170 Tb	250 Gb
$N_{max}=12$	250 M	4 Tb	60 Gb		

Space	Basis dim	matrix store (2-body)	factorization (2-body)	matrix store (3-body)	factorization (3-body)
$N_{shell}=3$	0.4 M	0.8 Gb	6 Mb	10 Gb	44 Mb
$N_{shell}=4$	45 M	330 Gb	0.3 Gb	9 Tb	4 Gb
$N_{shell}=5$	2 G	38 Tb	16 Gb	2 Pb	140 Gb
$N_{shell}=6$	50 G	2 Pb	87 Gb	170 Pb	3 Tb

Parallel Implementation

Factorization makes it easier to compute workload and distribute across multiple nodes



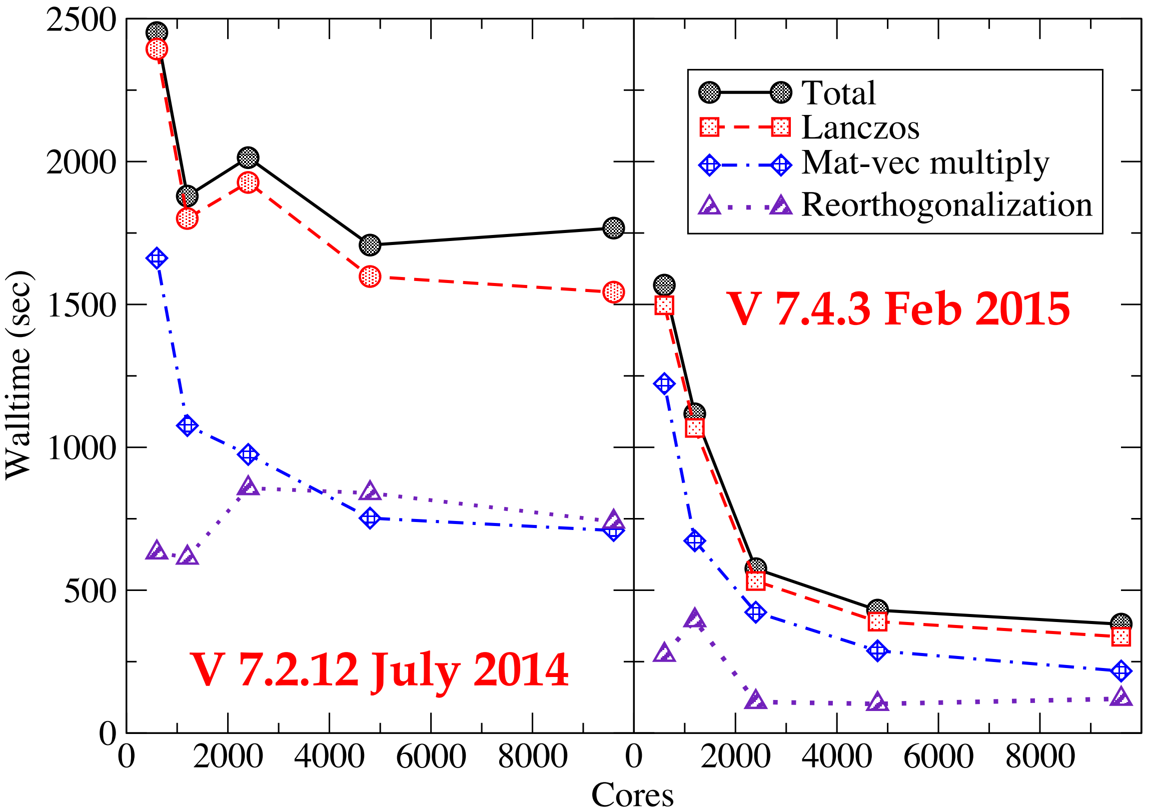


PARALLEL IMPLEMENTATION – LATEST DEVELOPMENTS

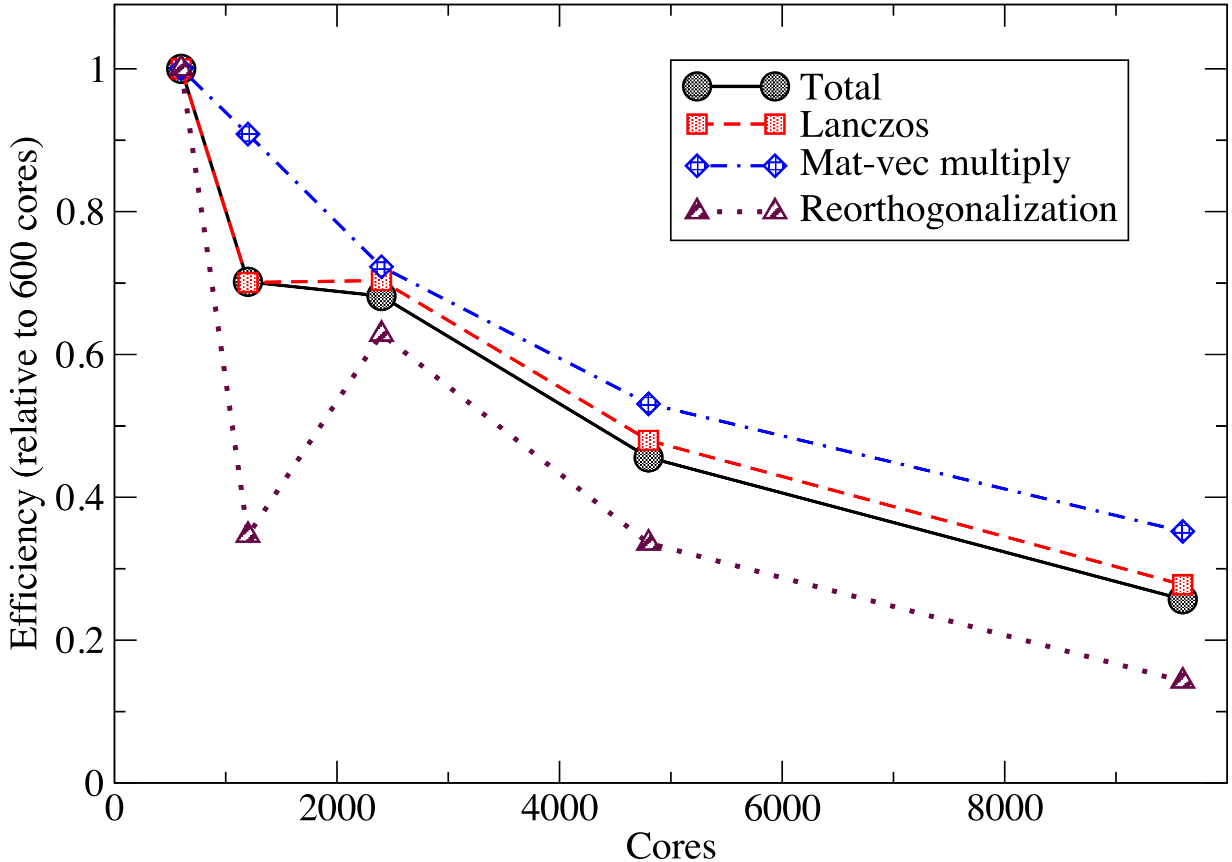
Over the past year we have dramatically improved our parallel performance (mostly through better use of MPI) due to Ken McElvain, UC Berkeley grad student

^{54}Mn in *pf* shell
(dim = 187 M)
200 iterations

LLNL Sierra



Strong scaling



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(dim = 187 M)
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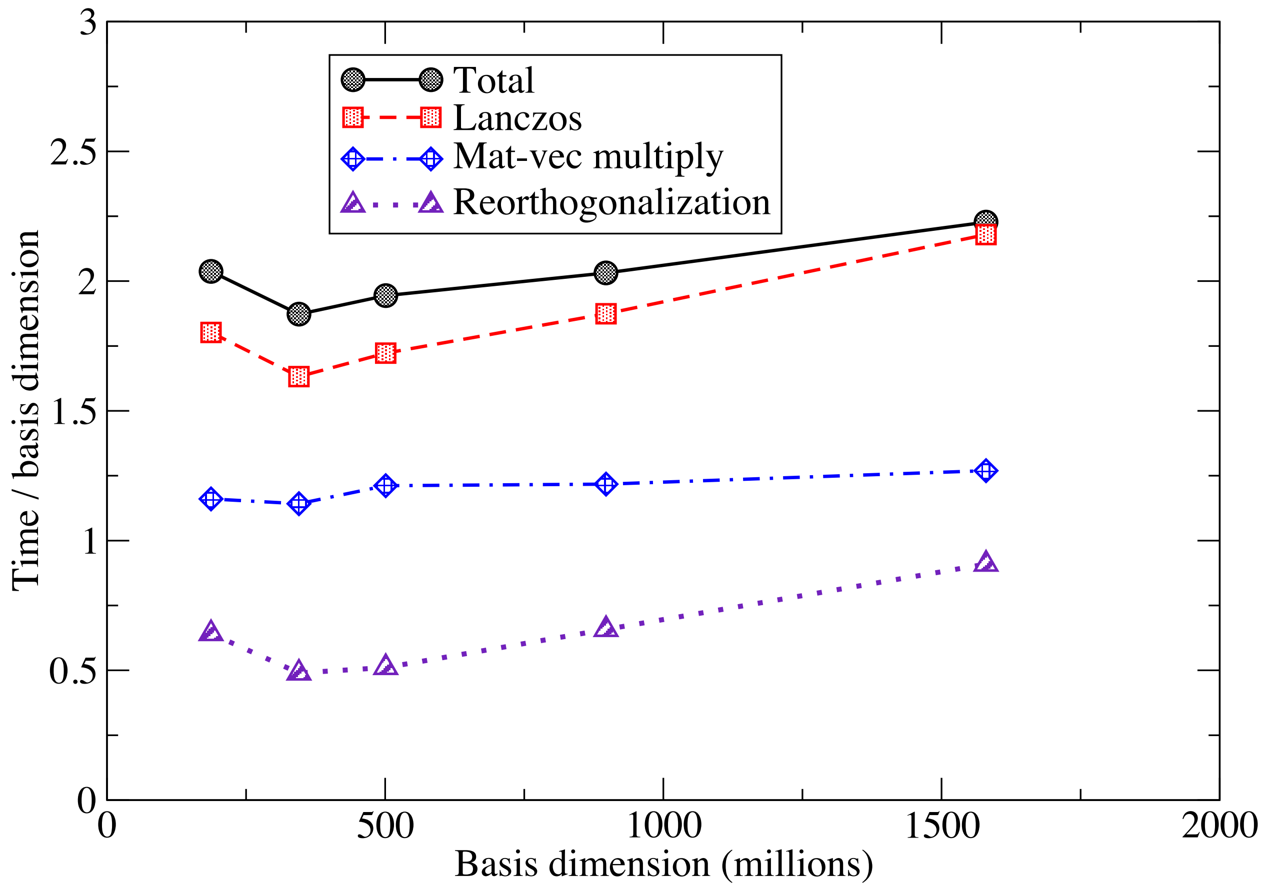
LLNL Sierra

V 7.4.3 Feb 2015

PARALLEL IMPLEMENTATION – LATEST DEVELOPMENTS



pf shell nuclides
(200 iterations)
800 MPI procs x 12 OpenMP threads

LLNL Sierra

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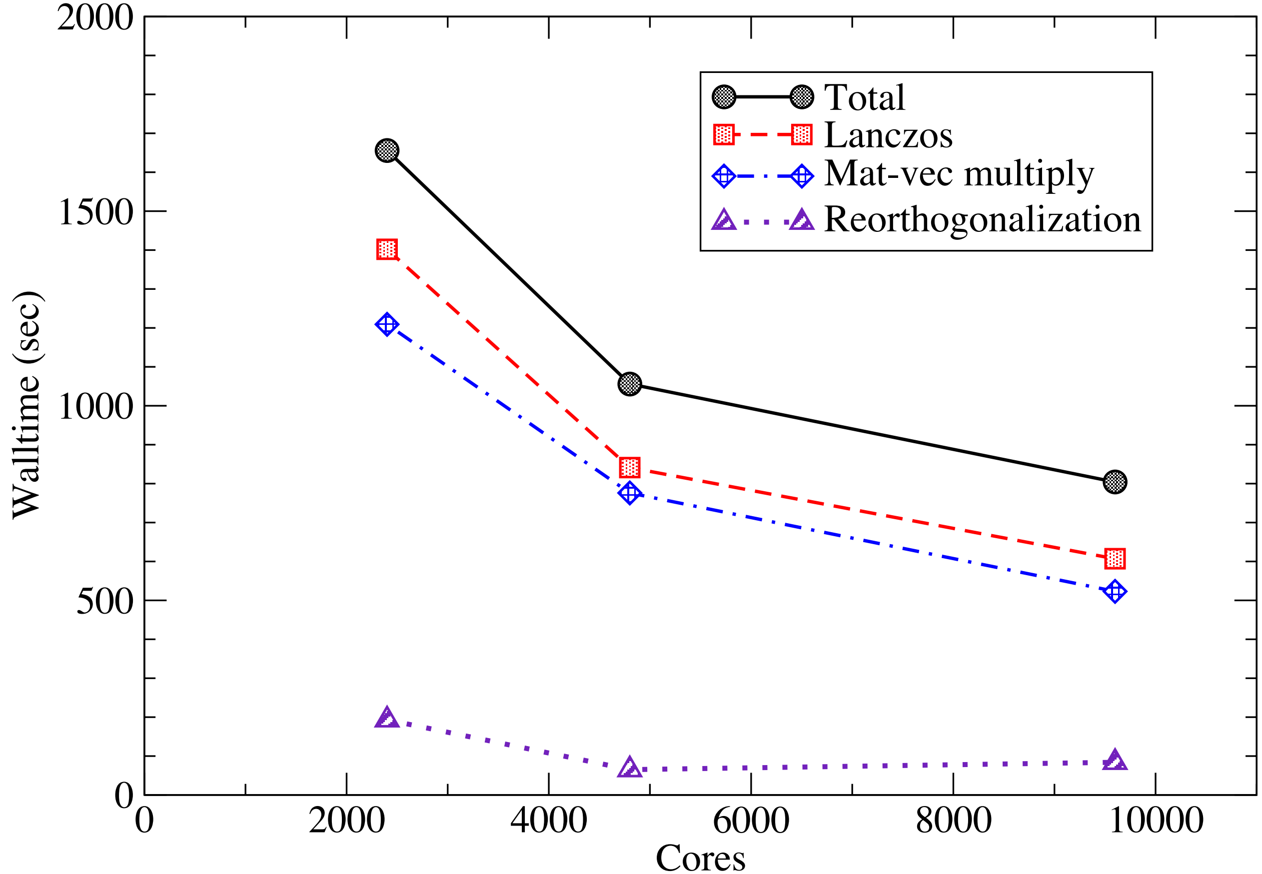
PARALLEL IMPLEMENTATION – LATEST DEVELOPMENTS



NCSM ^{10}B, N_{max} = 9 (dim = 547 M)
(100 iterations)
800 MPI procs x 12 OpenMP threads

LLNL Sierra

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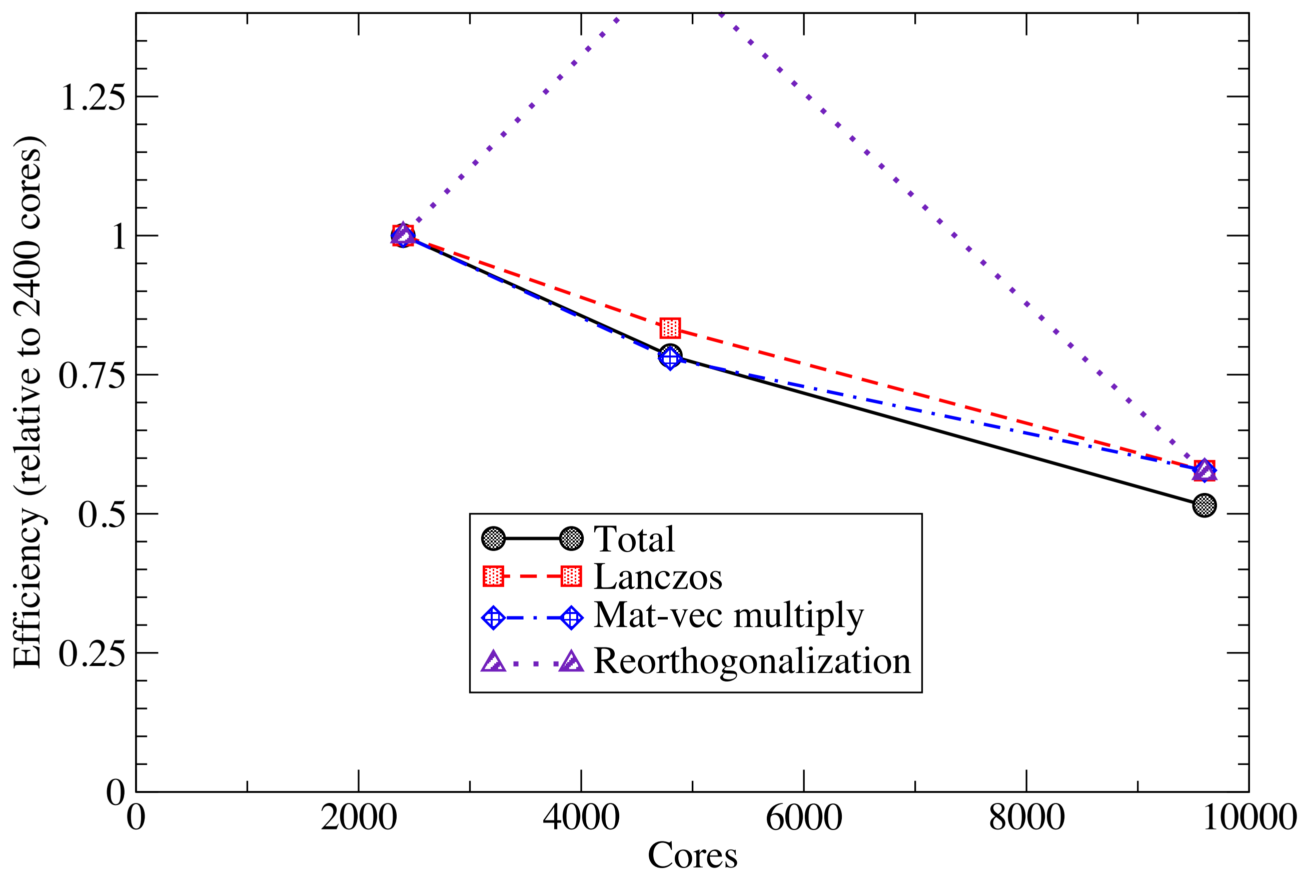
Strong scaling



NCSM ^{10}B, N_{max} = 9 (dim = 547 M)
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LLNL Sierra

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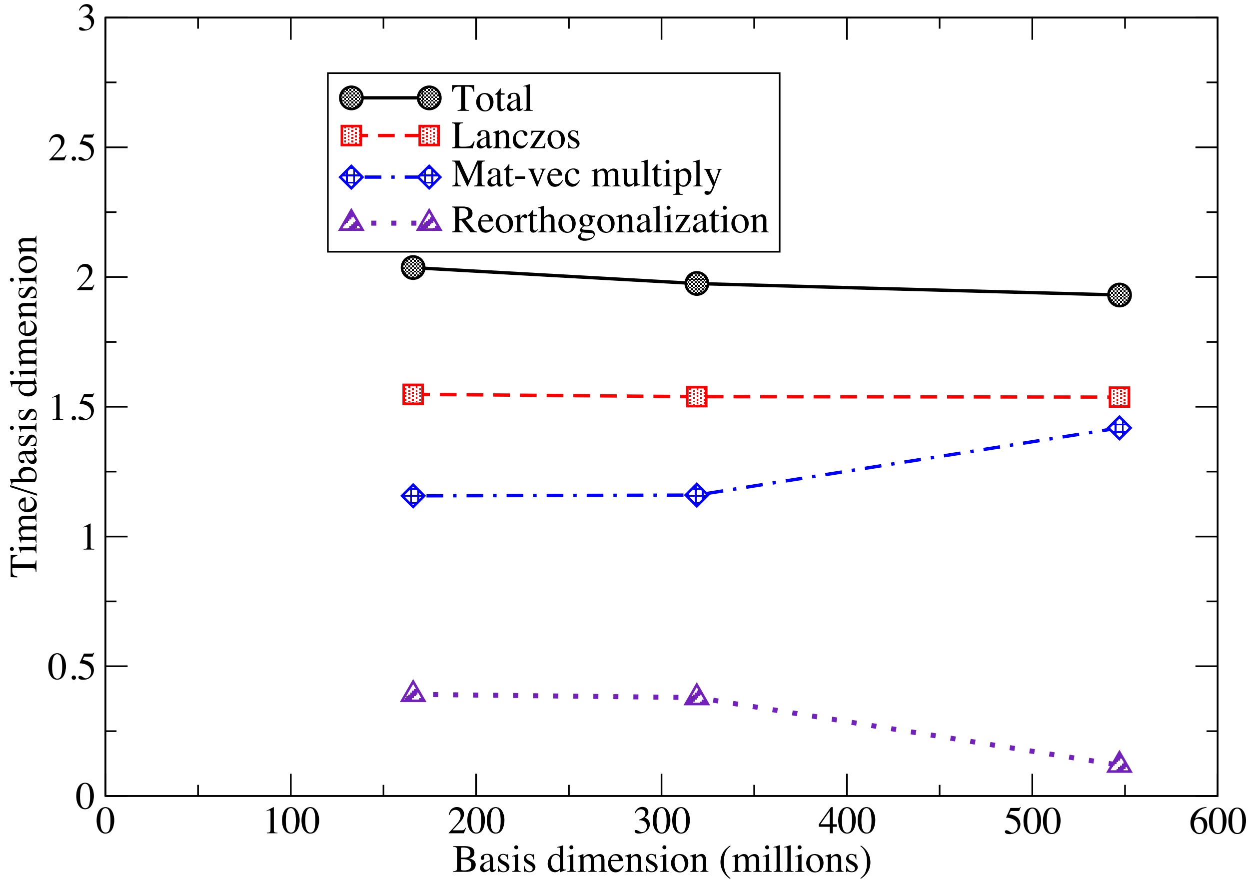
Parallel Implementation – Latest developments



NCSM *p*-shell nuclides
(100 iterations)
800 MPI procs x 12 OpenMP threads

LLNL Sierra

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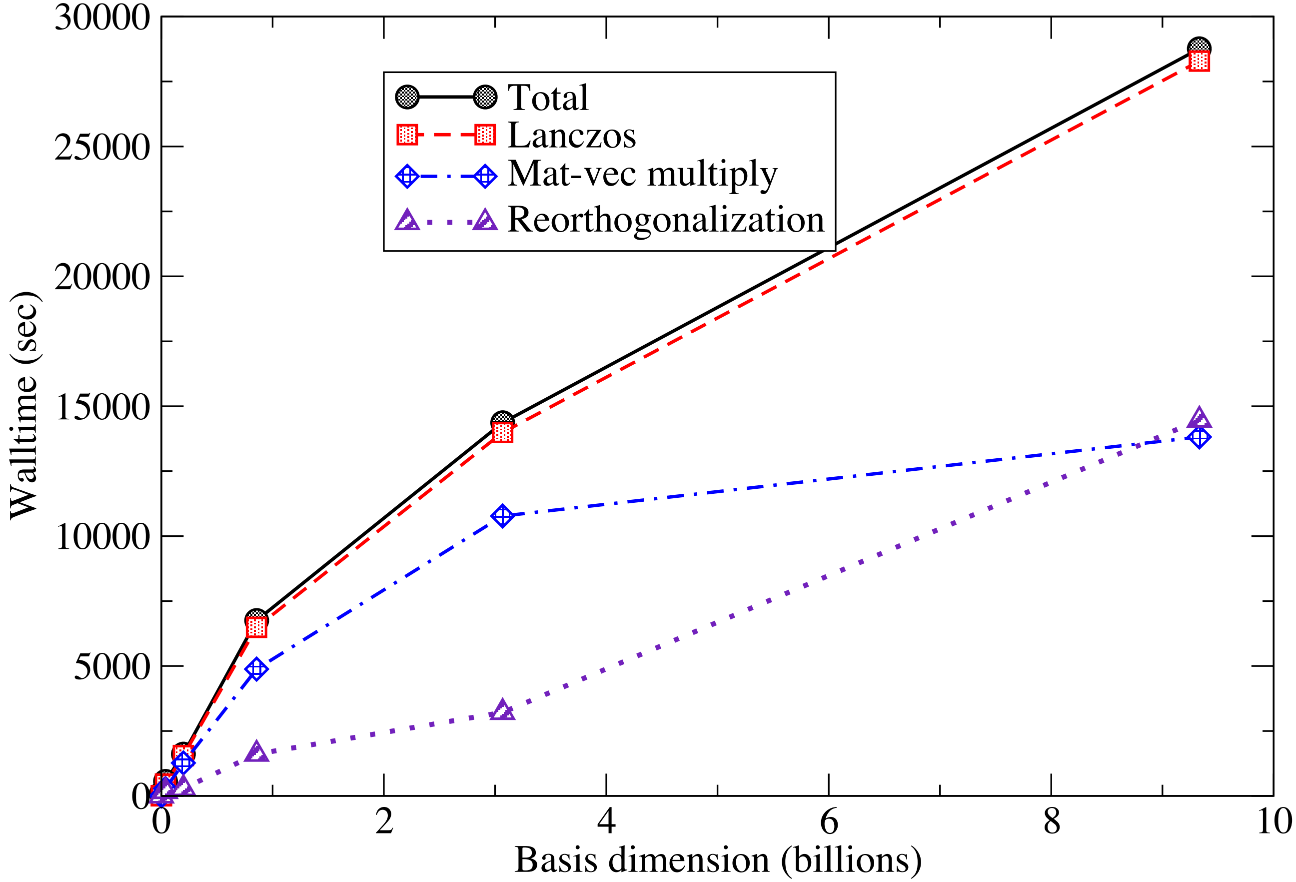
Parallel Implementation – Latest Developments

Science runs! Dark matter scattering cross-sections



Xe isotopes with ^{100}Sn core
(140-250 iterations)
6000-12000 MPI procs x 4-6 OpenMP threads

LBL/NERSC Edison

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FUTURE WORK

Improved memory load:

Because we chunk data based upon physics (quantum numbers), the natural distribution is irregular. Nonetheless we understand where and (mostly) how to improve the distribution of memory load:

- 2^{nd} generation fragmentation of Lanczos vectors (DONE)
- 2^{nd} generation distribution of "jump" arrays (almost finished)
- 2^{nd} generation storage of uncoupled matrix elements (in planning stage)

Improve work load balance:

We think we understand how and why the work load balance loses efficiency: different ordering of loops and irregular loop sizes. We are gathering data (H. Shan, LBL).

Pushing to larger cases

We plan to go to dim ~ 24 billion this summer(< 6000 MPI nodes)

We plan to go to dim ~ 100 billion in the next year

"It's not enough to just show up. You have to have a business plan."

Applications

Applications

IIa: Transitions and the Brink-Axel hypothesis

+ Michael K. G. Kruse (LLNL), W. Erich Ormand (LLNL), and Micah Schuster (SDSU)

Transitions and the Brink-Axel hypothesis

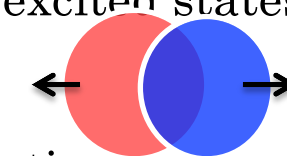
+ Michael K. G. Kruse (LLNL), W. Erich Ormand (LLNL), and Micah Schuster (SDSU)

Brink-Axel hypothesis (D. Brink, D. Phil. thesis, Oxford University (unpublished), 1955; P. Axel, Phys. Rev. **126**, 671 (1962)):

If the ground state has a giant dipole resonance (GDR), then excited states should have GDR

and

because the GDR is a collective proton-versus-neutrons oscillations, the GDR should be insensitive to the initial state.



Electric dipole

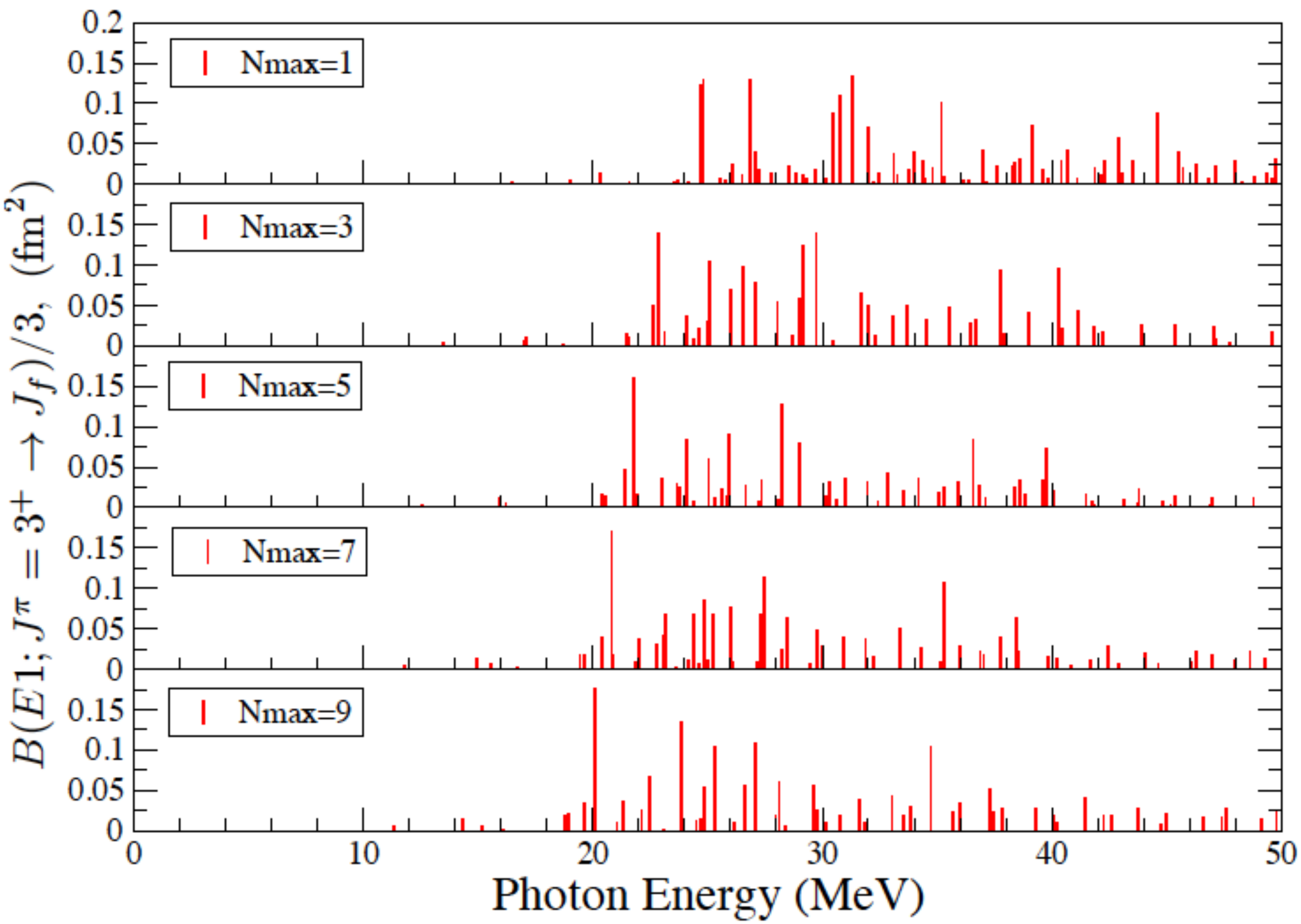
$$S(E_i, E_x) = \sum_f \left|\langle f|\hat{T}|i\rangle\right| \delta(E_x - E_f + E_i)$$

"Transition strength function"

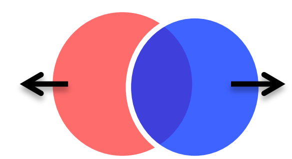
Brink-Axel: "S(E_i,E_x) independent of E_i"

Large Scale Shell-Model Calculations for Open-shell nuclei

Kruse, Ormand, and Johnson: arXiv:1502:03464



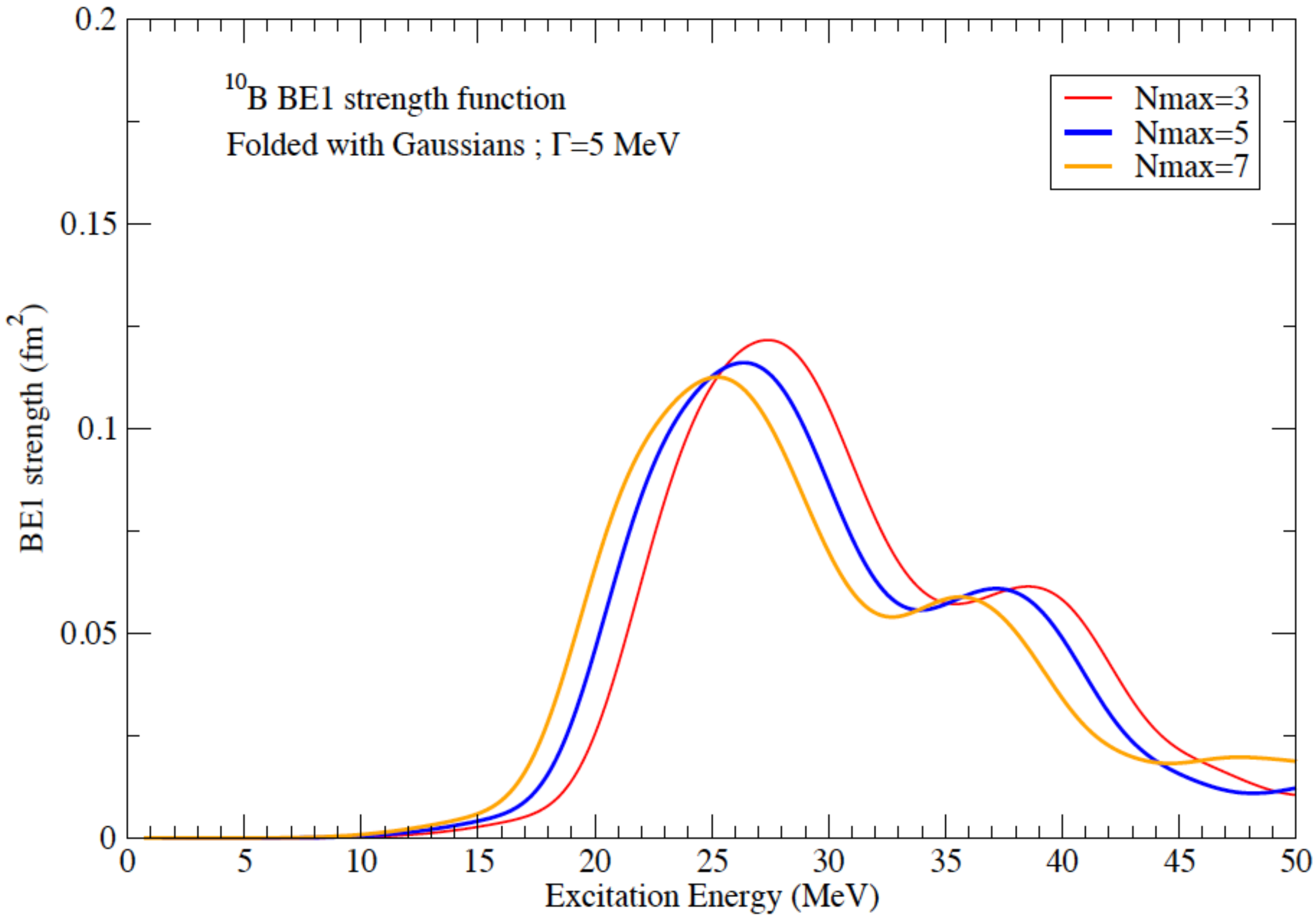
^{10}B E1 response



Electric dipole

Large Scale Shell-Model Calculations for Open-shell nuclei

BE1 strength with increasing basis size



Strength distribution shape is robust in Nmax.

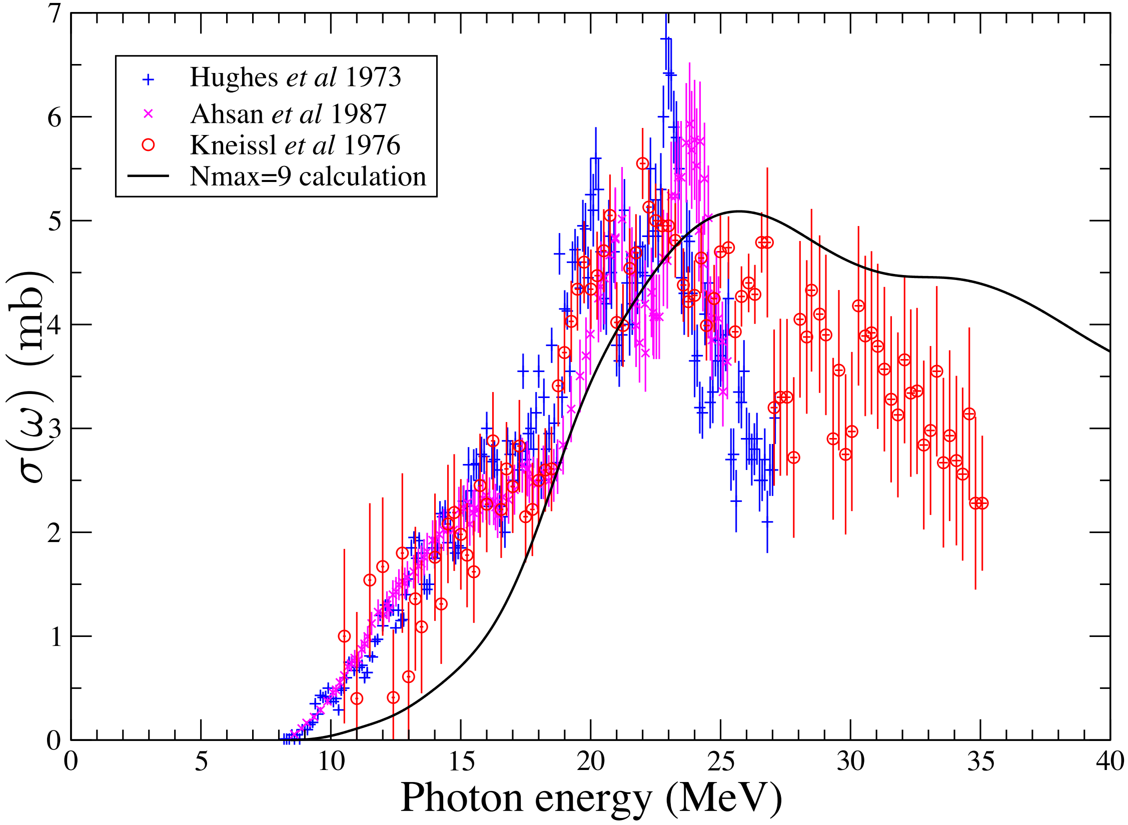
Slowly moves down in energy as a function of Nmax.

How to extrapolate this distribution?

Perhaps it is best to extrapolate centroids?

Large Scale Shell-Model Calculations for Open-shell nuclei

Kruse, Ormand, and Johnson: arXiv:1502:03464



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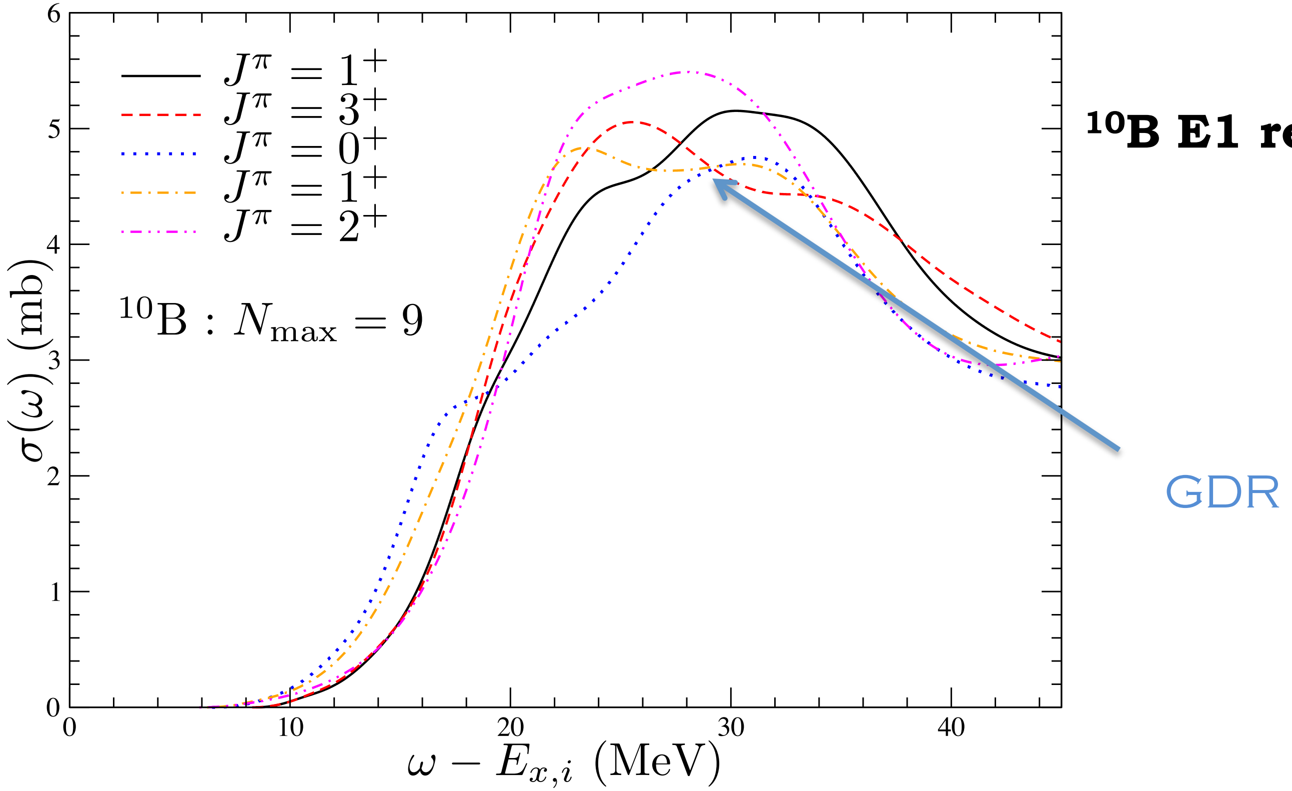
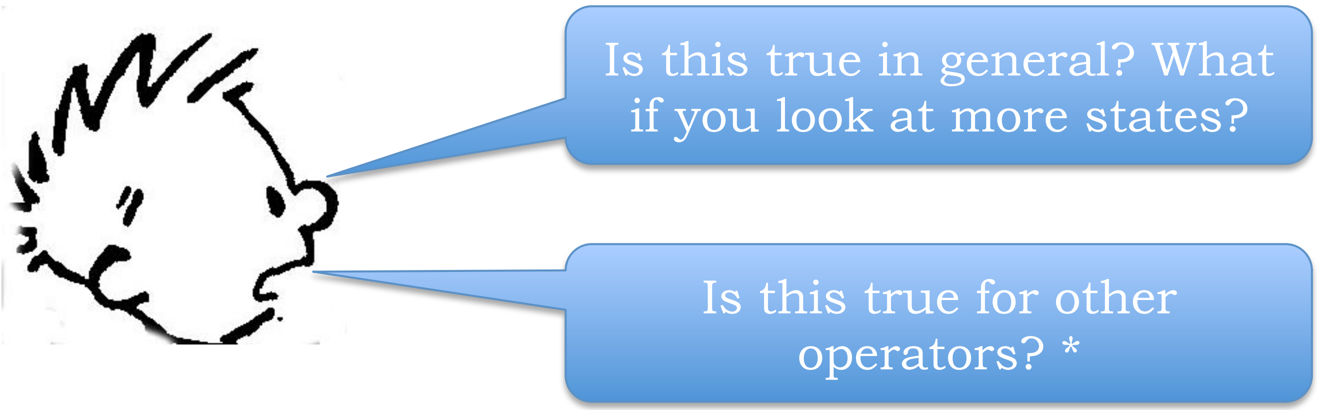


^{10}B E1 response

Brink-Axel: "S(E_i,E_x) independent of E_i"

Large Scale Shell-Model Calculations for Open-shell nuclei



* Some evidence to the contrary (with Gamow-Teller operator): Frazier, Brown, Millener, and Zelevinsky, Phys. Lett B **414**, 7 (1997); Misch, Fuller, and Brown, PRC 90, 065808 (2014)

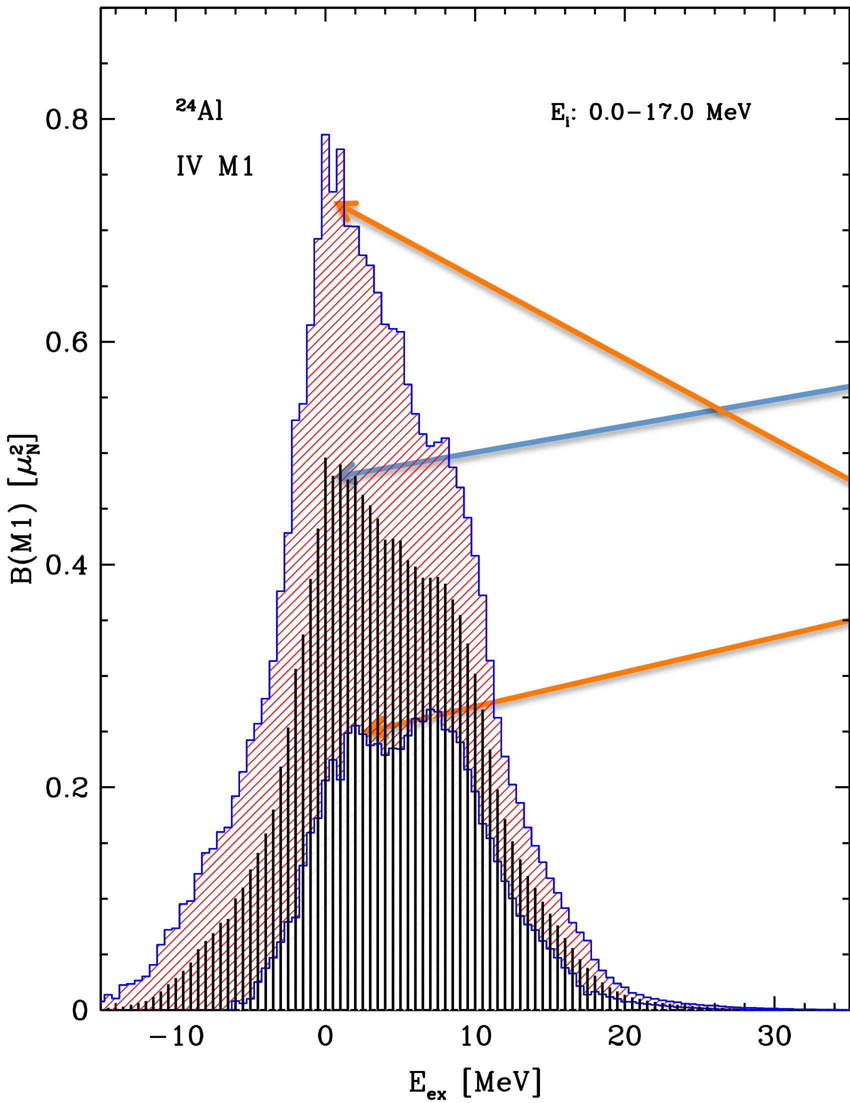
Large Scale Shell-Model Calculations for Open-shell nuclei

Some preliminary work by Micah Schuster: phenomenological calculations in *sd*-shell where we can compute hundreds of initial states

Took energy bins of initial states, computed strength functions, and computed average strength function + fluctuations about average

Large Scale Shell-Model Calculations for Open-shell nuclei

Took energy bins of initial states, computed strength functions, and computed average strength function + fluctuations about average



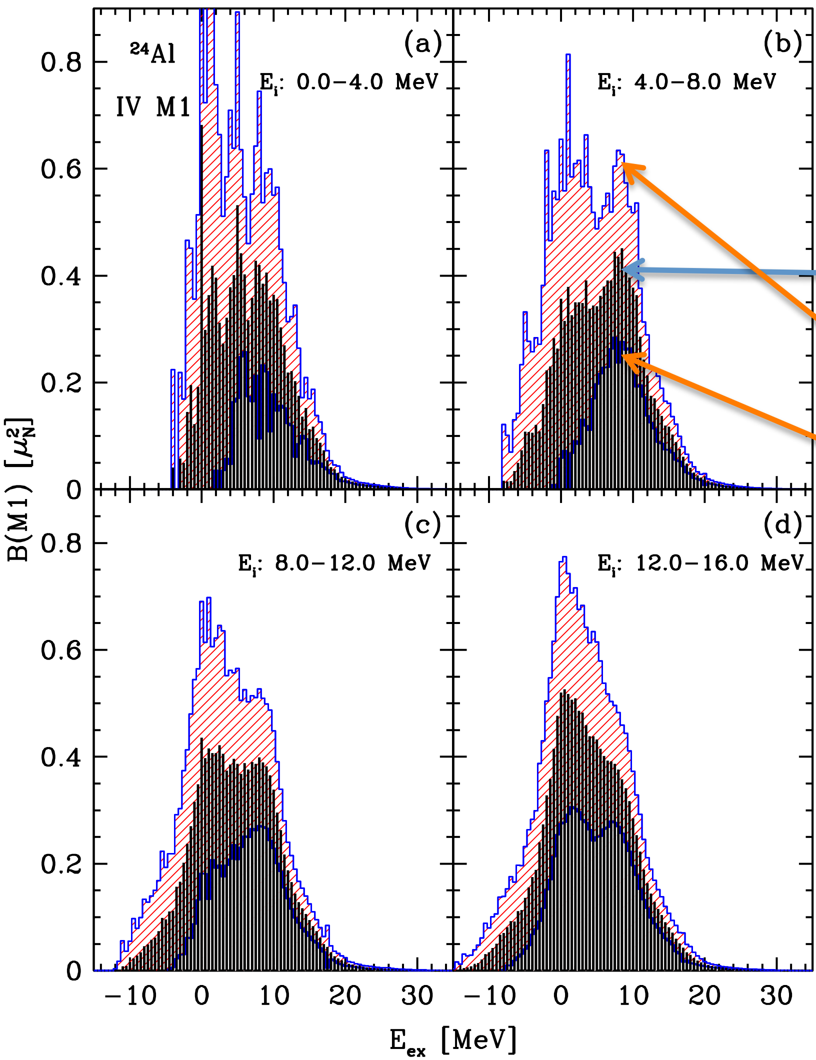
^{24}Al with isovector M1

Average strength function

1 std. dev. fluctuation about average

Large Scale Shell-Model Calculations for Open-shell nuclei

Took energy bins of initial states, computed strength functions, and computed average strength function + fluctuations about average



^{24}Al with isovector M1

Average strength function

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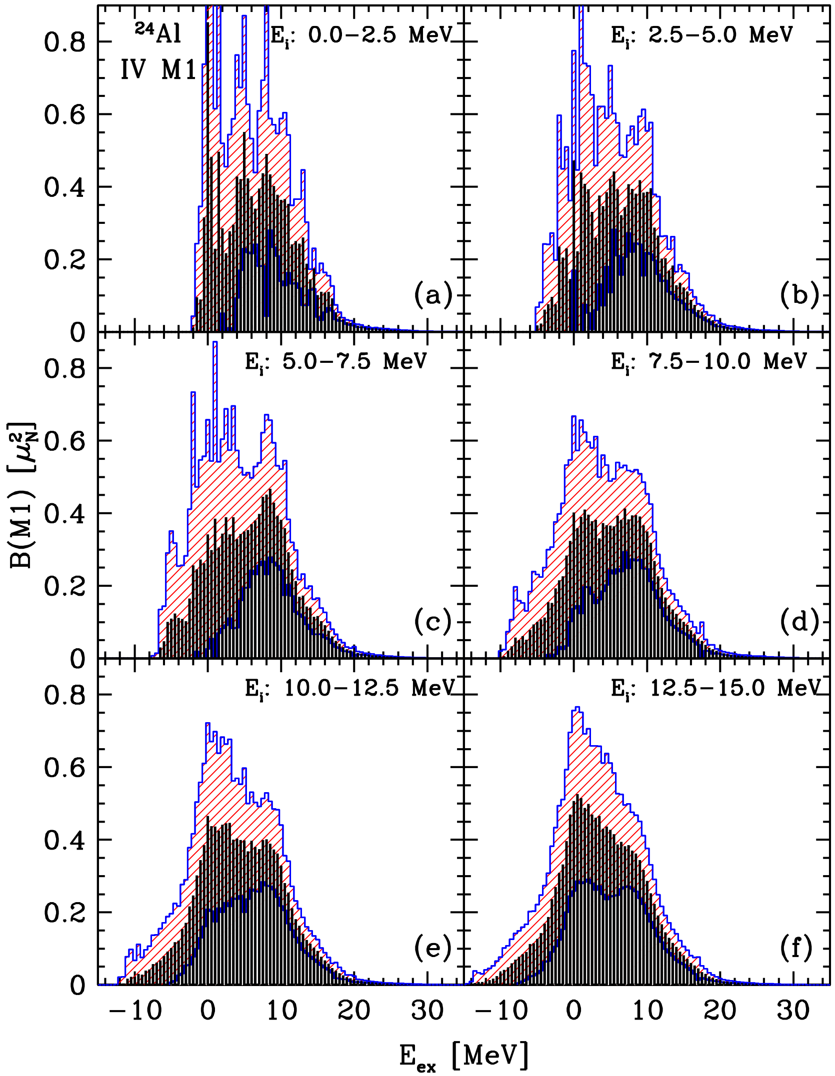
Large Scale Shell-Model Calculations for Open-shell nuclei

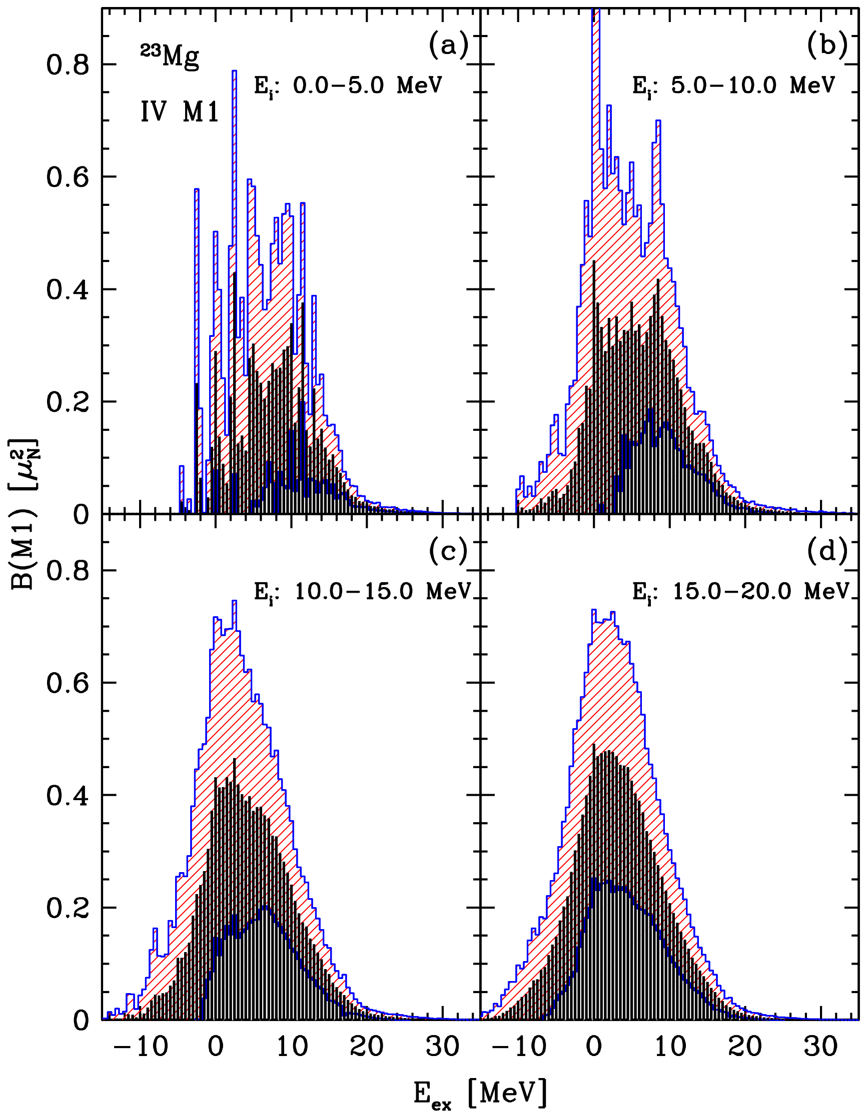
Took energy bins of initial states, computed strength functions, and computed average strength function + fluctuations about average



^{24}Al with isovector M1

Large Scale Shell-Model Calculations for Open-shell nuclei

Looks like large fluctuations about the average; can we characterize / quantify this?



^{23}Mg with isovector M1

Large Scale Shell-Model Calculations for Open-shell nuclei

The total strength
(or *non-energy-weighted sum rule*)
can be computed as a simple expectation value

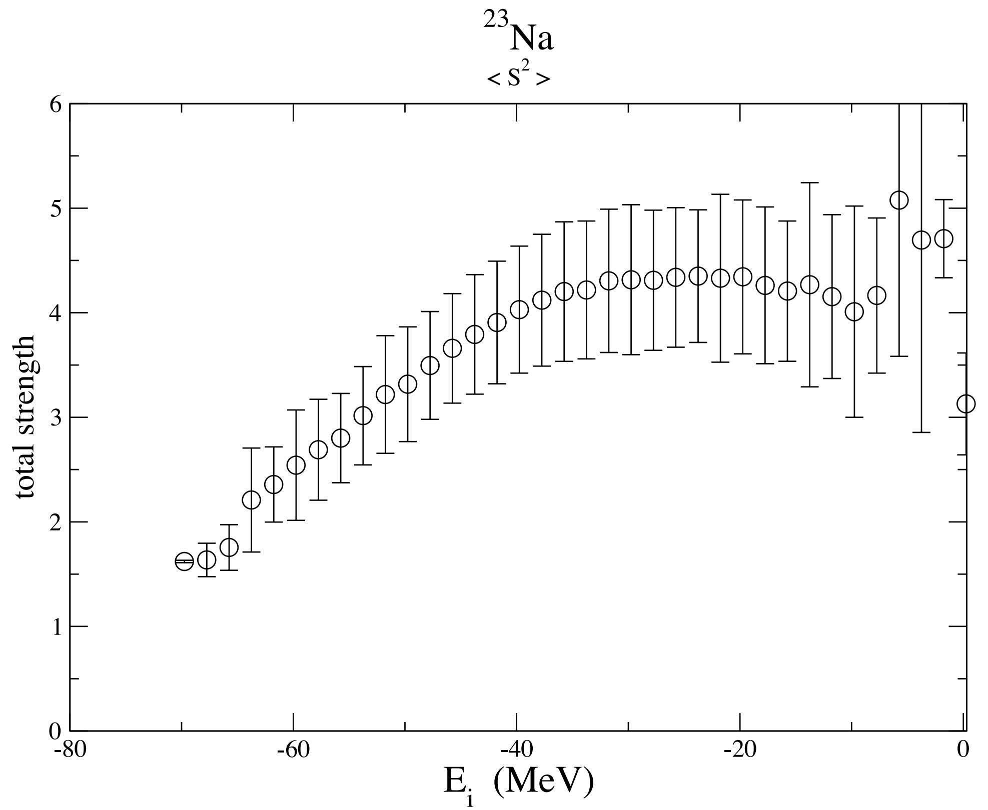
$$S_0(E_i) = \int S(E_i, E_x)\, dE_x = \sum_f \left| \langle f | \hat{T} | i \rangle \right| = \langle i | \hat{T}^+ T | i \rangle$$

Looks like large fluctuations about the average; can we characterize / quantify this?

Large Scale Shell-Model Calculations for Open-shell nuclei

The total strength (or *non-energy-weighted sum rule*)

$$\int S(E_i, E_x) dE_x = \sum \left| \langle f | \hat{T} | i \rangle \right| = \langle i | \hat{T}^{+} T | i \rangle$$



Large Scale Shell-Model Calculations for Open-shell nuclei

Furthermore, the smooth secular behavior is easily understood through *spectral distribution theory* of J. B. French *et al*

Average expectation value is just a trace!

$$\langle \hat{O} \rangle = \frac{1}{N} \sum_i \langle i | O | i \rangle = \frac{1}{N}\, tr\,(\hat{O})$$

Large Scale Shell-Model Calculations for Open-shell nuclei

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(Linear) energy dependence is *also* a trace!

$$\frac{1}{N}\sum_i E_i \langle i|O|i\rangle = \frac{1}{N}\sum_i \langle i|OH|i\rangle = \frac{1}{N}\, tr\,(\widehat{OH})$$

Slope is given by $< O\, H > - < O > < H >$

Large Scale Shell-Model Calculations for Open-shell nuclei

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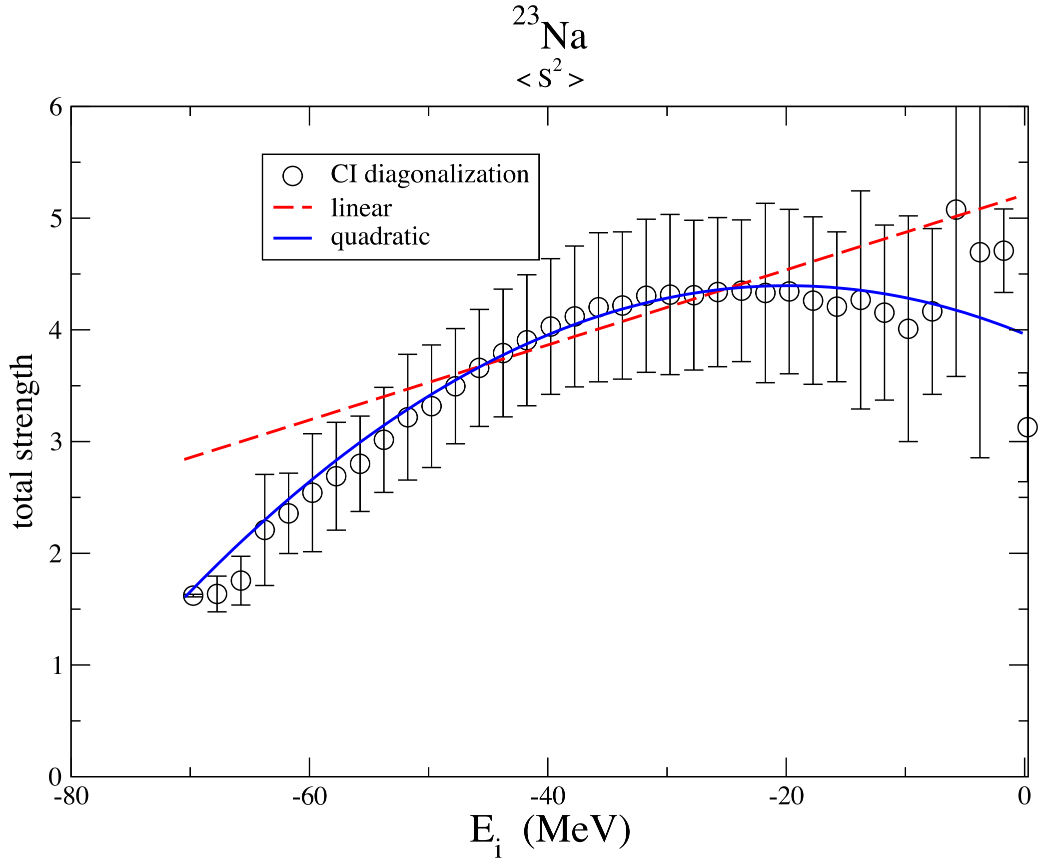
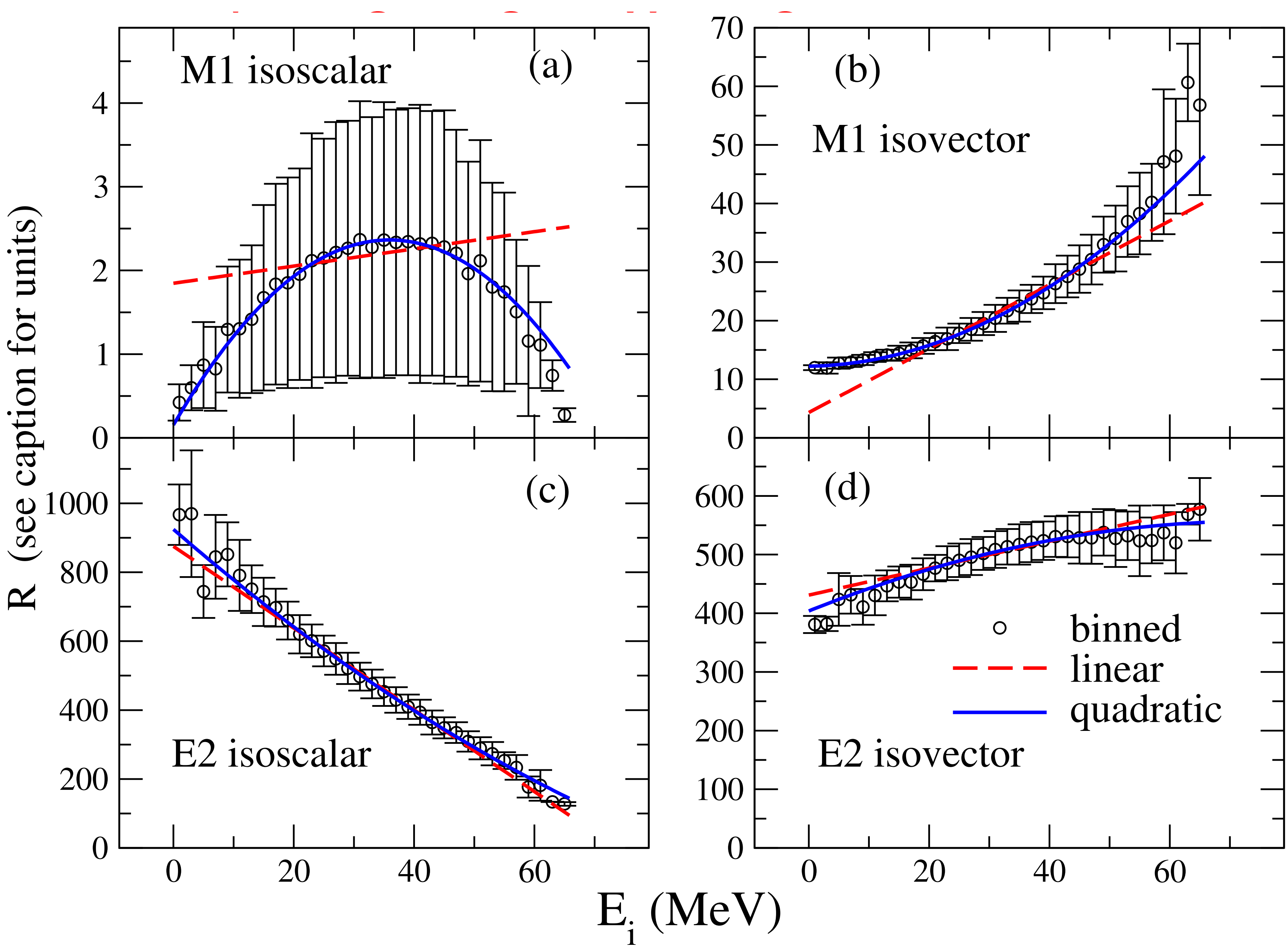
$$\frac{1}{N} \sum_i E_i \langle i | O | i \rangle = \frac{1}{N} \sum_i \langle i | OH | i \rangle = \frac{1}{N} \, tr \, (\widehat{OH})$$

From this we can derive the secular behavior of expectation values

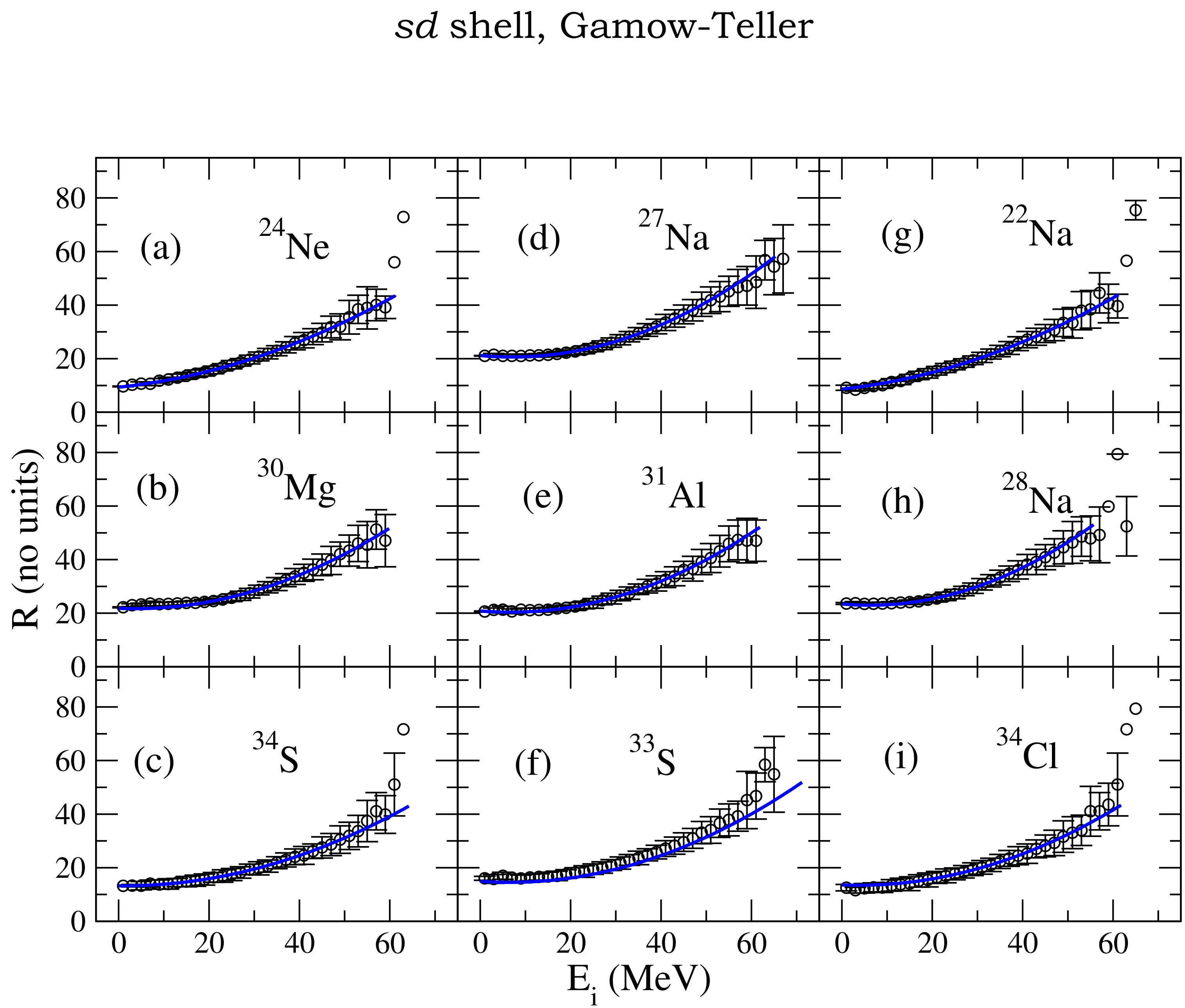
Large Scale Shell-Model Calculations for Open-shell nuclei

Furthermore, the smooth secular behavior is easily understood through *spectral distribution theory* of J. B. French *et al*

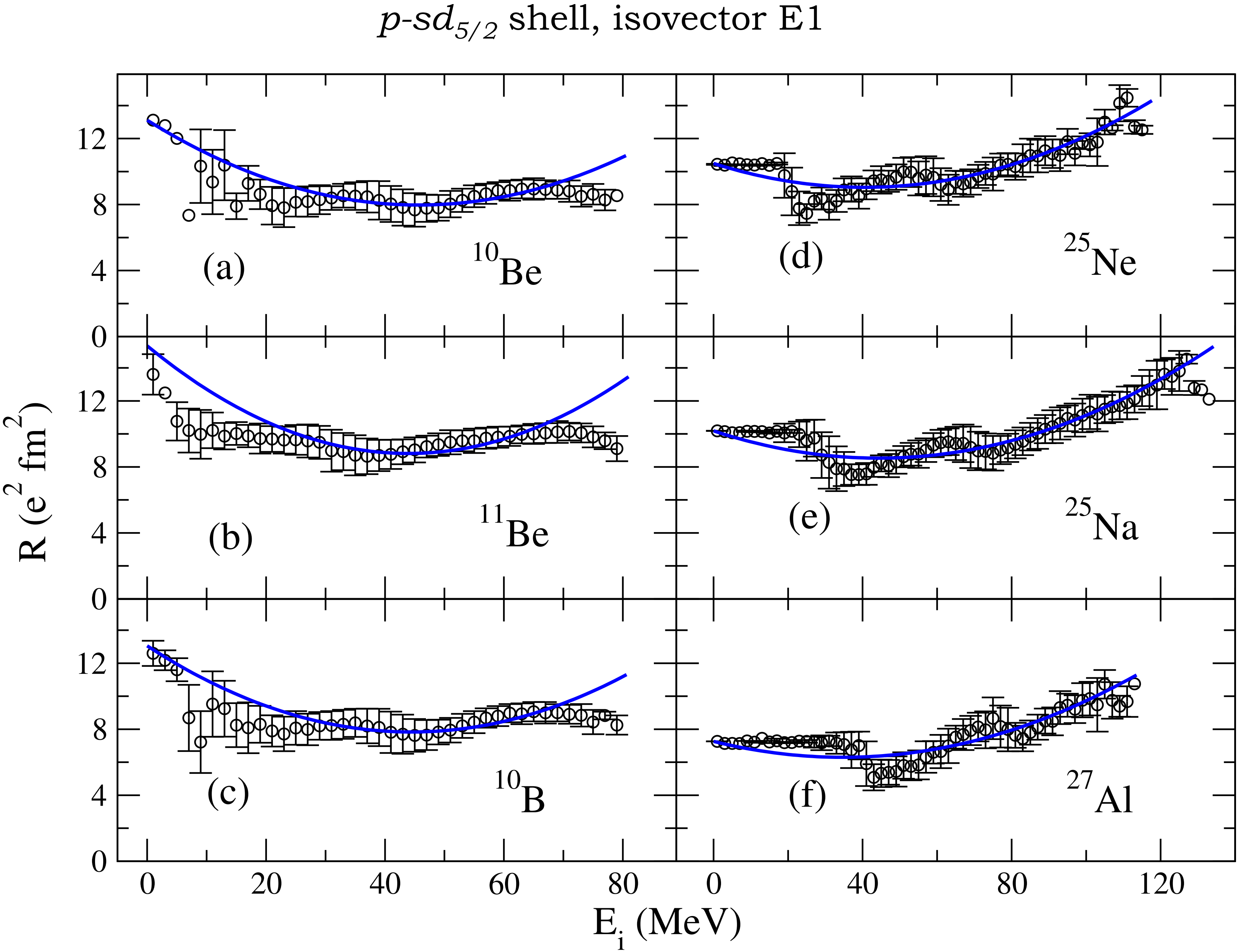




M1 isoscalar
(a)
(b)
M1 isovector
(c)
(d)
E2 isoscalar
E2 isovector
binned
linear
quadratic
R (see caption for units)
E_i (MeV)



sd shell, Gamow-Teller
R (no units)
E_i (MeV)
(a) 24Ne
(b) 30Mg
(c) 34S
(d) 27Na
(e) 31Al
(f) 33S
(g) 22Na
(h) 28Na
(i) 34Cl
0
20
40
60
80



p-sd5/2 shell, isovector E1
R (e2 fm2)
Ei (MeV)
(a)
10Be
(b)
11Be
(c)
10B
(d)
25Ne
(e)
25Na
(f)
27Al
0
4
8
12
0
20
40
60
80
120

Large Scale Shell-Model Calculations for Open-shell nuclei

The generalized Brink-Axel hypothesis (for arbitrary operators) is *wrong*!

-- total strength evolves with initial (parent) energy

-- significant fluctuations even for nearby parent states

We can understand this through *spectral distribution theory*,

that is,

traces of operators (weighted by the energy);

A lack of energy dependence can occur *only* if

$$\langle O H \rangle - \langle O \rangle \langle H \rangle = 0$$

Applications

IIb: : *ab initio* Gamow-Teller transitions

Large Scale Shell-Model Calculations for Open-shell nuclei

Part IIb: *ab initio* Gamow-Teller transitions

- Gamow-Teller important for weak physics, astrophysics
- Avoids dependence on radial wavefunctions (at lowest order); mostly SU(4) irreps; Ikeda sum rule strong constraint
- Consistent quenching of coupling—exchange currents, or what?
- **What about 0-neutrino double-beta decay?**

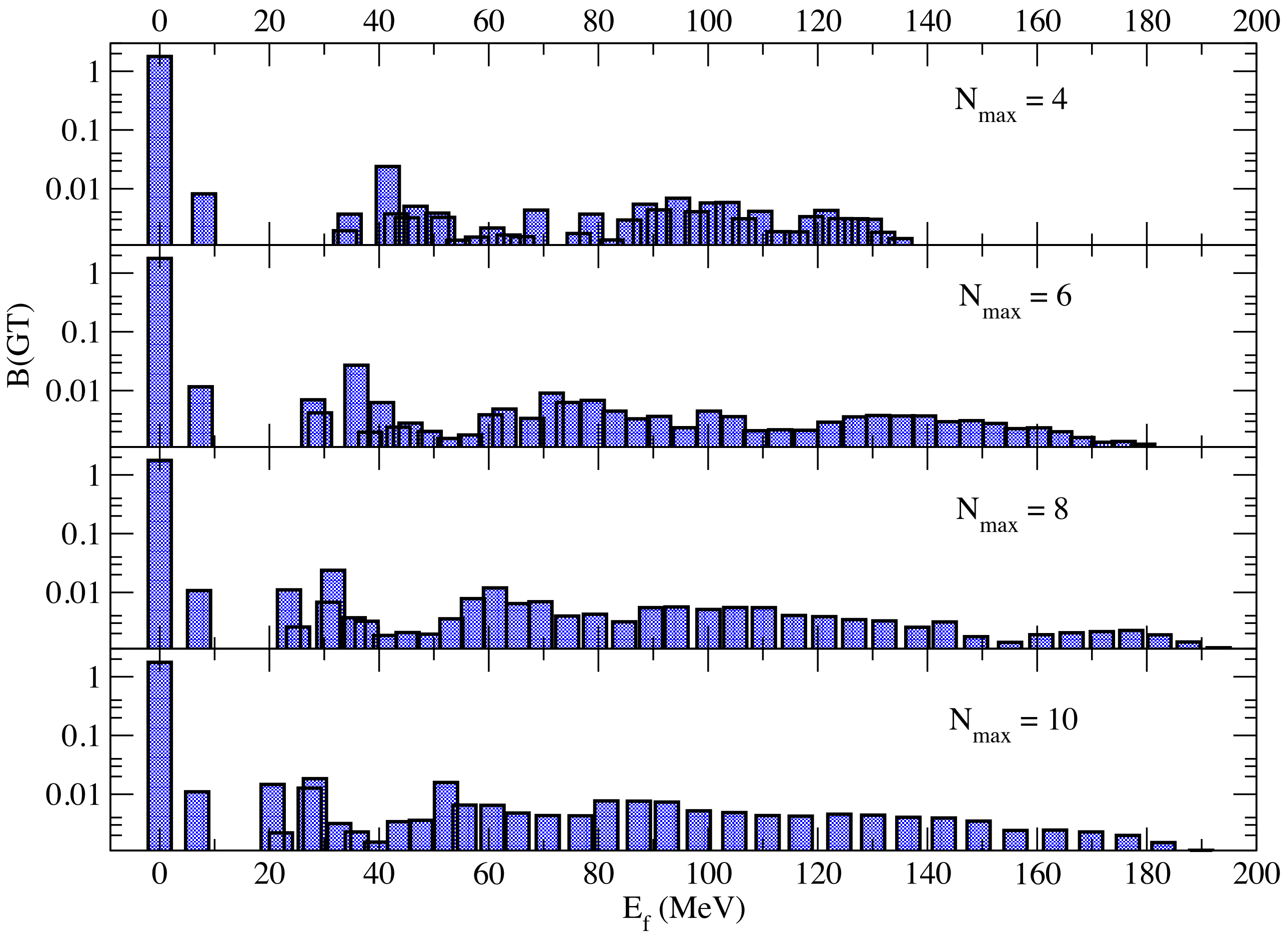
Two recent highlights:

Anomalously long ^{14}C half-life (Maris, Vary, Navratil, Ormand, Nam, Dean) Phys. Rev. Lett. 106, 202502 (2011): ‘accidental’ cancellation of matrix elements driven by 3-body force

Exchange current corrections from EFT (quenching of about 0.8):
S. Vaintraub, N. Barnea, and D. Gazit, Phys. Rev. C **79**, 065501 (2009);
J. Menendez, D. Gazit, and A. Schwenk, Phys. Rev. Lett **107**, 062501 (2011)

Large Scale Shell-Model Calculations for Open-shell nuclei

$^6He \rightarrow {}^6Li$

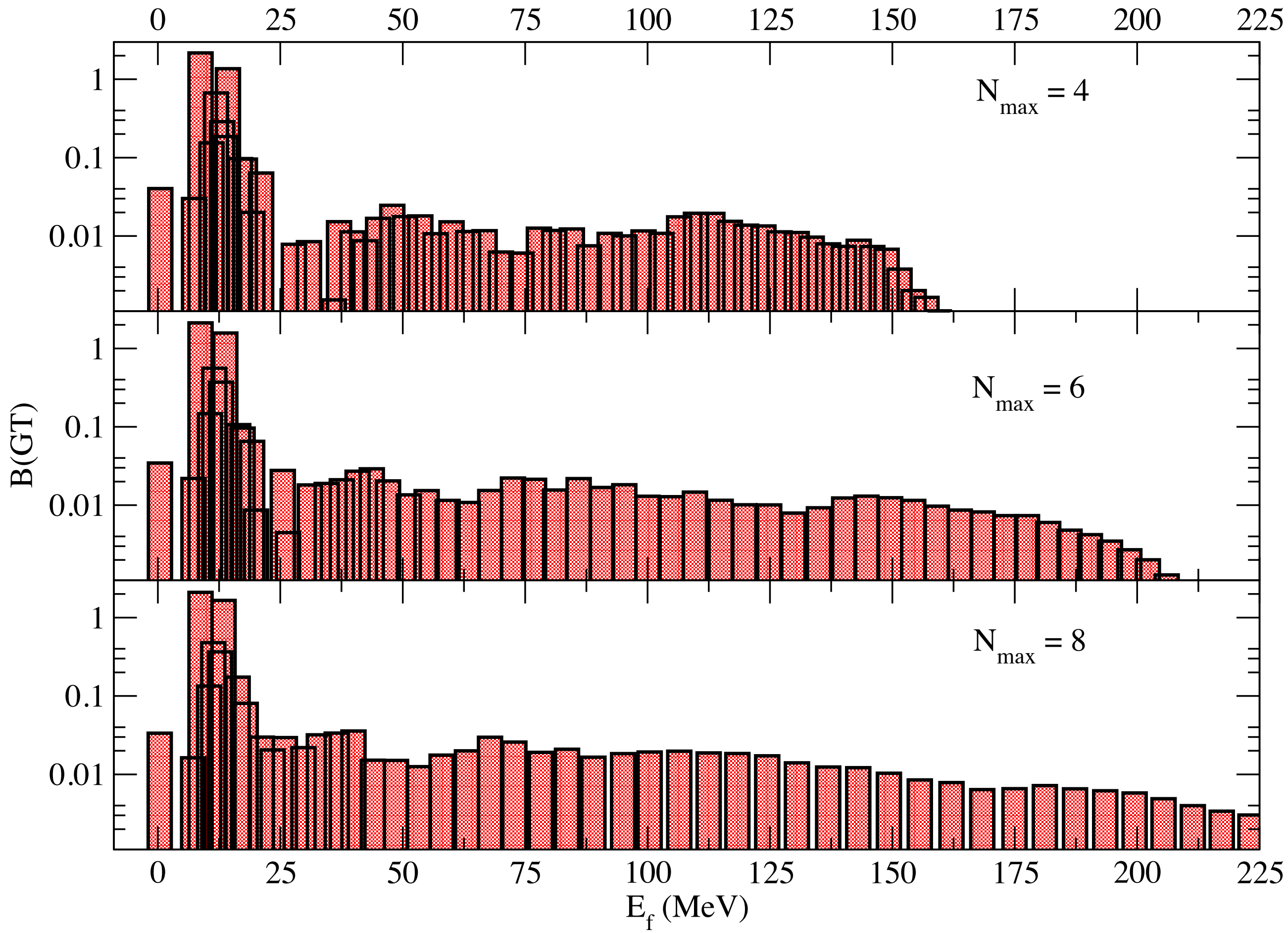


Preliminary!

Chiral 2-body forces SRG evolved to λ=2 fm^{-1})

Large Scale Shell-Model Calculations for Open-shell nuclei

^{7}He ➔ ^{7}Li

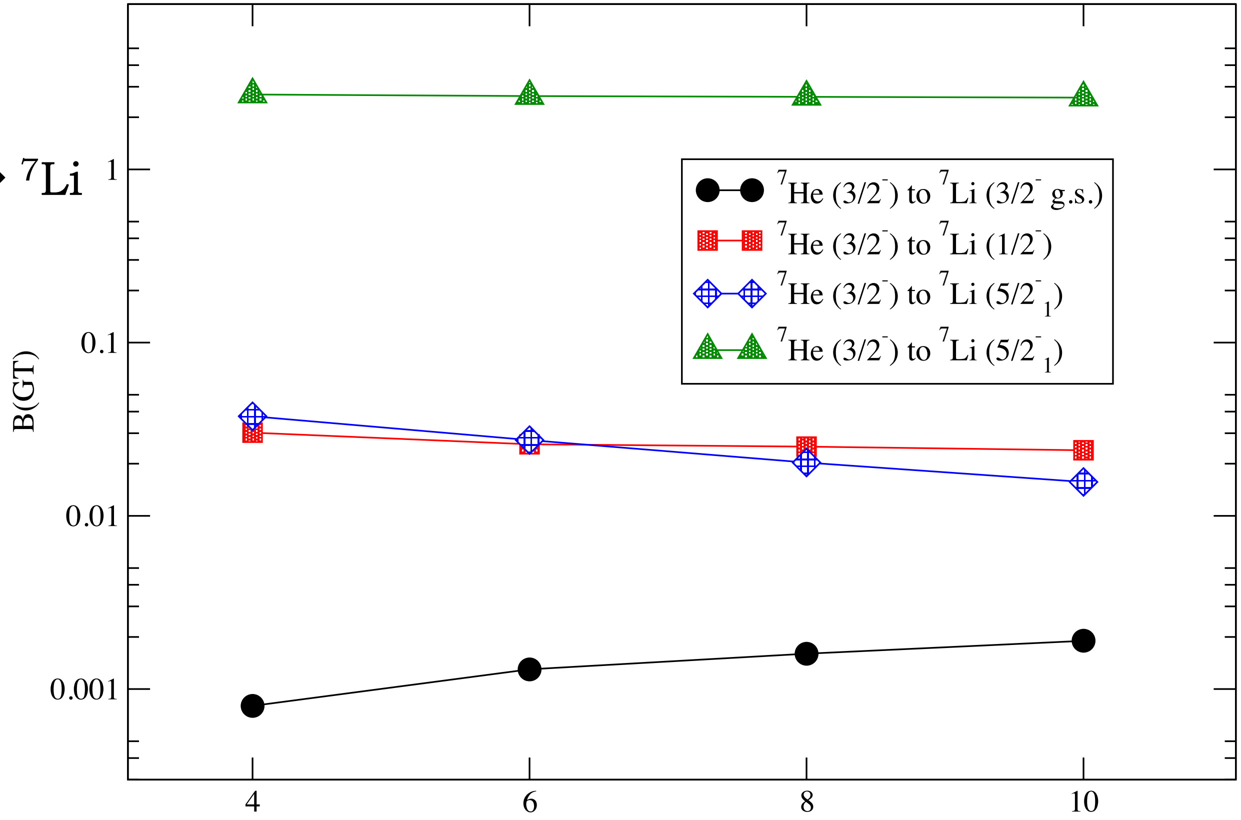


Preliminary!

(Run on desktop machine with BIGSTICK)

Large Scale Shell-Model Calculations for Open-shell nuclei

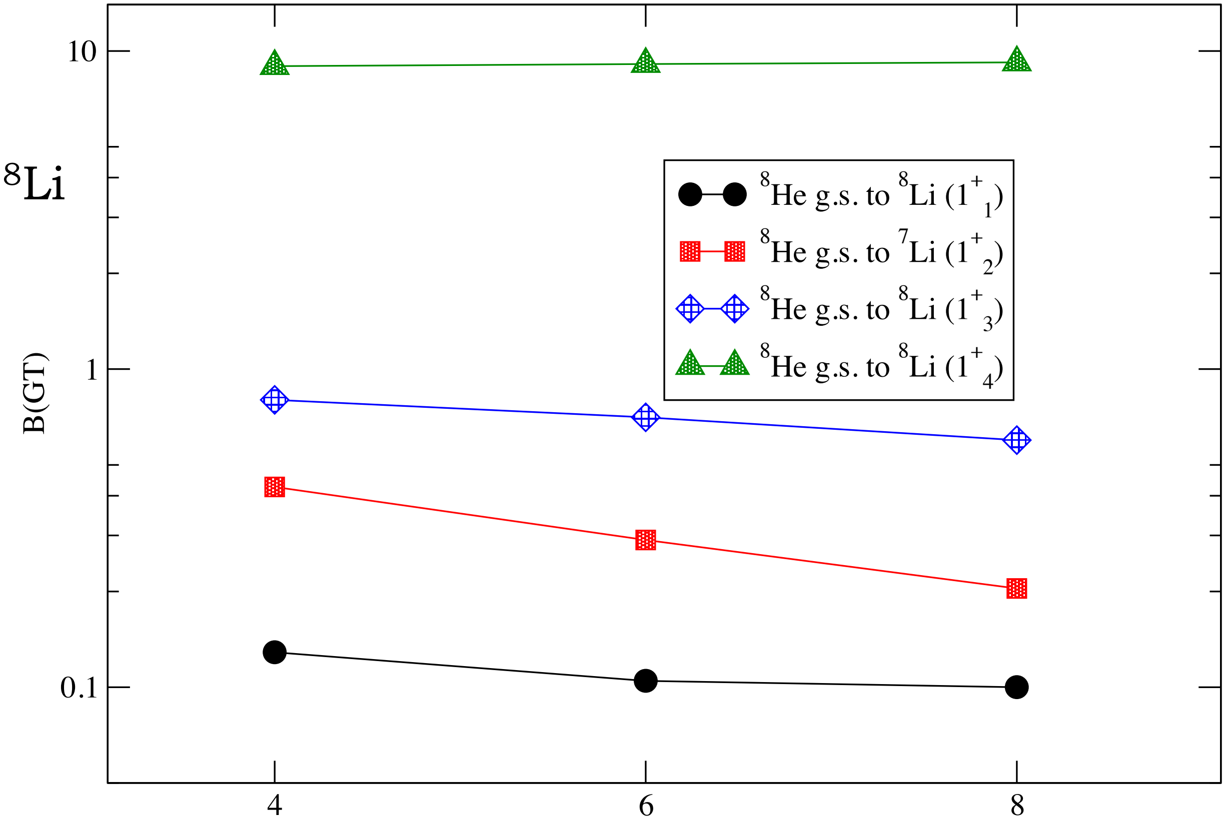
$^7He \rightarrow {}^7Li$



Preliminary!

Large Scale Shell-Model Calculations for Open-shell nuclei

$^8He \rightarrow ^8Li$



Preliminary!

Large Scale Shell-Model Calculations for Open-shell nuclei

Need to run higher N_{max} (on supercomputers) but …

Despite being a "simple" operator, transition matrix elements of Gamow-Teller ($\sigma\tau$) do not have simple behavior:

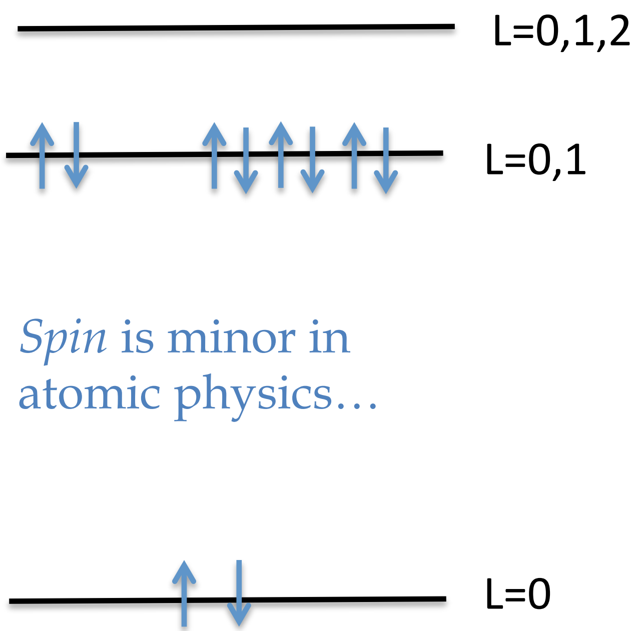
- Some transitions quickly converge as we go up in N_{max}, others not
- Should be investigated by doing L-S/SU(4) decomposition
- Effect of 3-body forces likely important
- More work on chiral EFT exchange forces should be done
- Likely strong implications for $0\nu-\beta\beta$ matrix elements…

APPLICATIONS

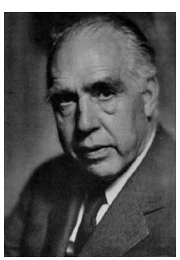
IIc: :Spin-orbit decomposition of *ab initio* nuclides

C. W. J, Phys. Rev. C **91**, 034313 (2015).

Atoms :

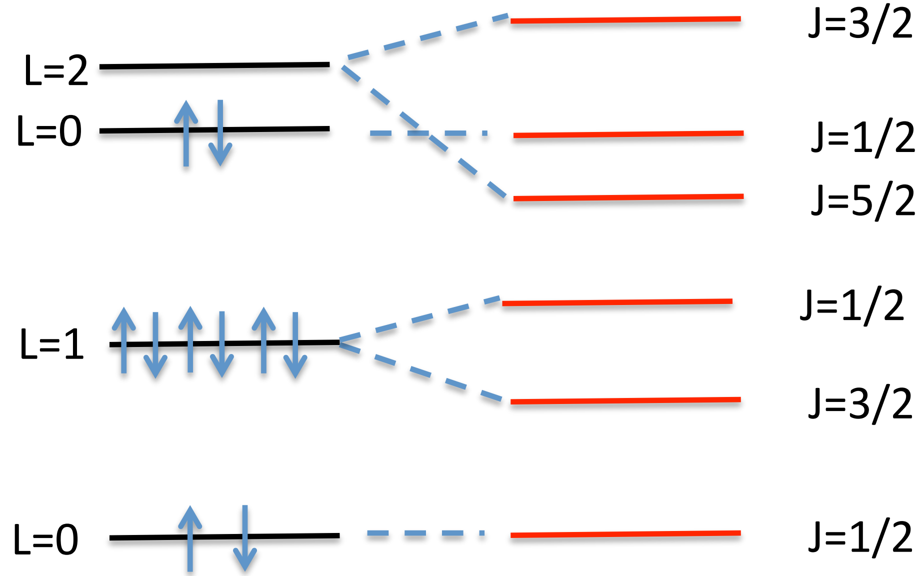


Spin is minor in atomic physics…




(Niels Bohr) (E. Schrodinger)

Nuclei:



…but crucial in nuclear physics…

(Maria Goeppert-Mayer)

Large Scale Shell-Model Calculations for Open-shell nuclei

j-j versus L-S

$$\begin{array}{ccccccccc} l_1 & & l_2 & & l_3 & & l_4 & & \\ + & & + & & + & & + & & \dots \\ s_1 & & s_2 & & s_3 & & s_4 & & \\ = & & = & & = & & = & & \\ j_1 & + & j_2 & + & j_3 & + & j_4 & + & \dots \end{array} = J$$

"j-j coupling"

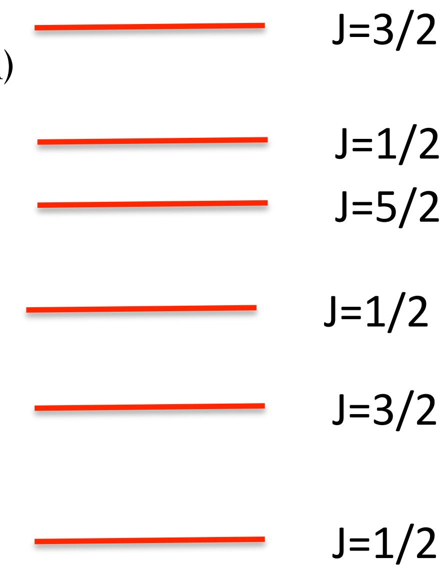
$$\begin{array}{c} l_1 + l_2 + l_3 + l_4 + \dots \\ s_1 + s_2 + s_3 + s_4 + \dots \end{array} \begin{array}{c} = L \\ + \\ = S \end{array} = J$$

"L-S coupling"

How good is j-j coupling?

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

Nuclei:



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 % $(0p_{3/2})^4$

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)

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% $(0d_{5/2})^6 (1s_{1/2})^2$	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 % $(0d_{5/2})^{12} (1s_{1/2})^4$	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.

Let's now do L-S decomposition of *ab initio* *p*-shell wavefunctions

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?

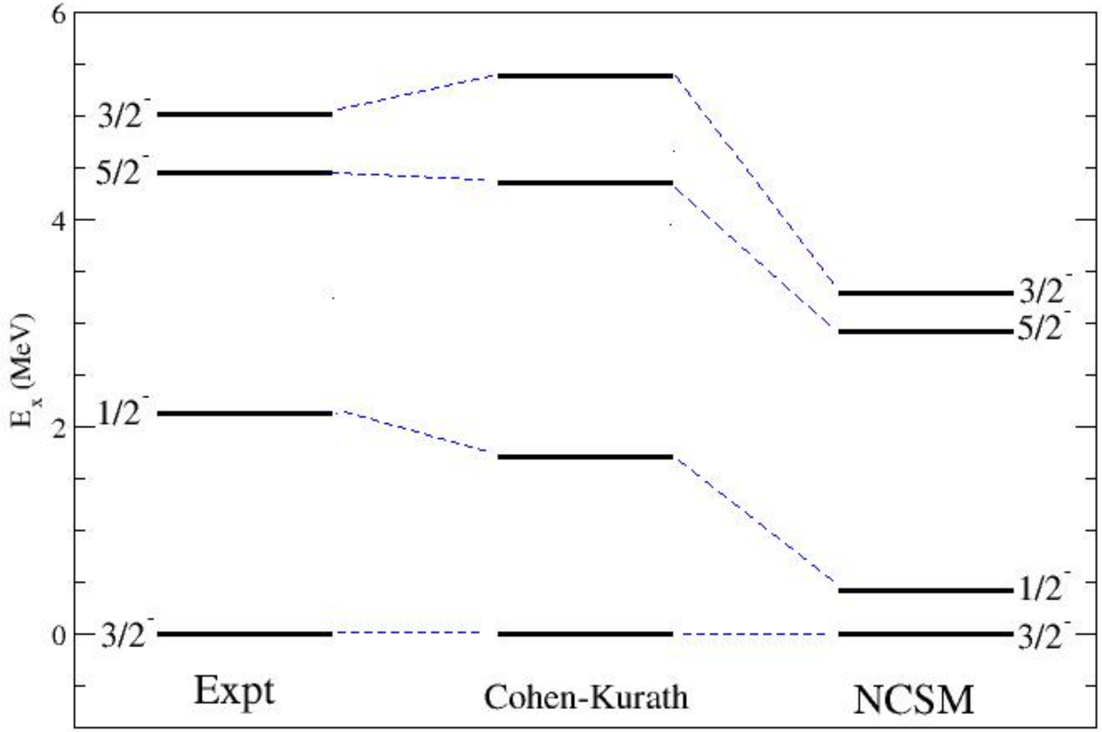
Note: In this talk I only give 2-body results. 3-body forces later…

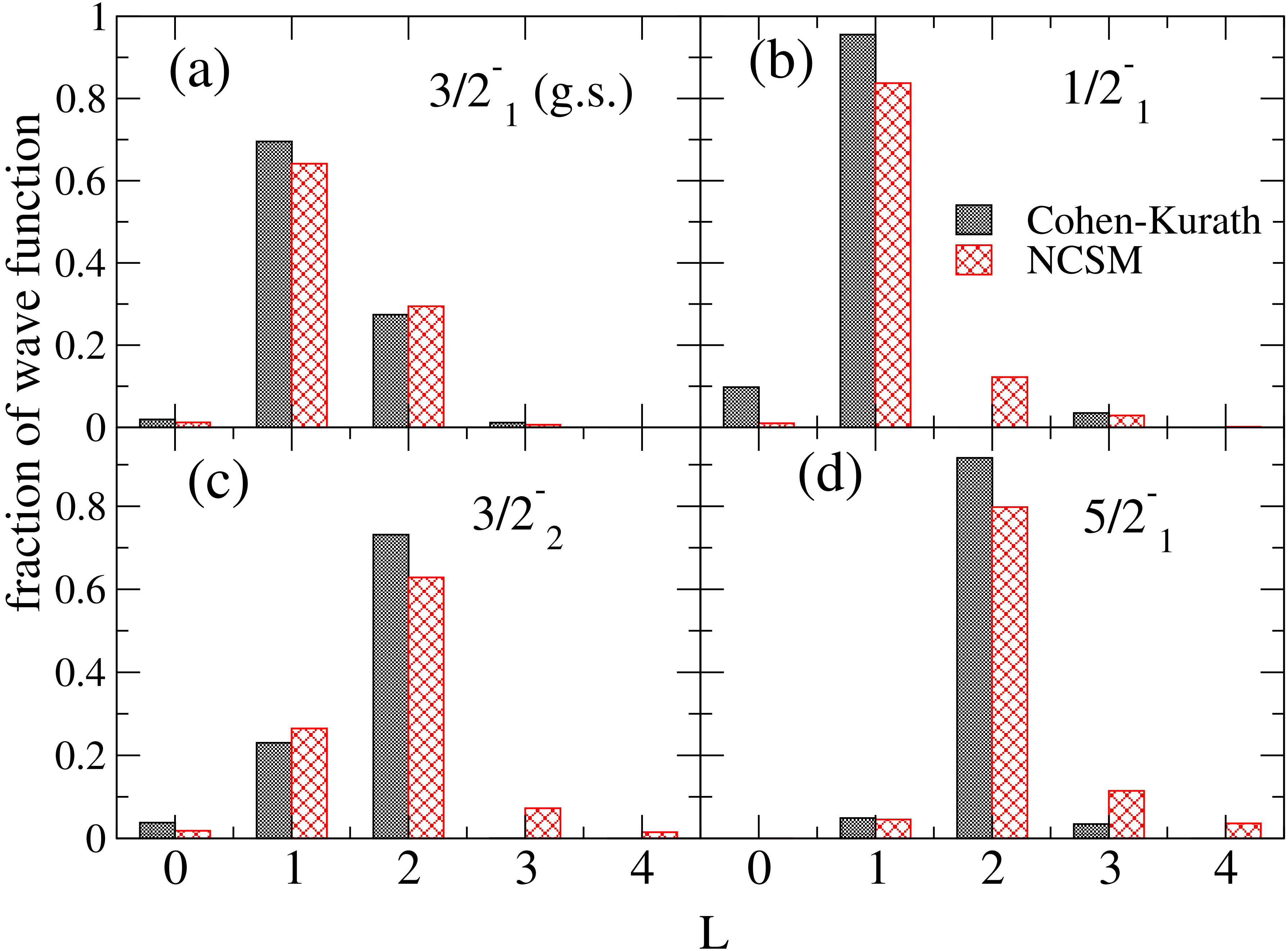
Large Scale Shell-Model Calculations for Open-shell nuclei

^{11}B

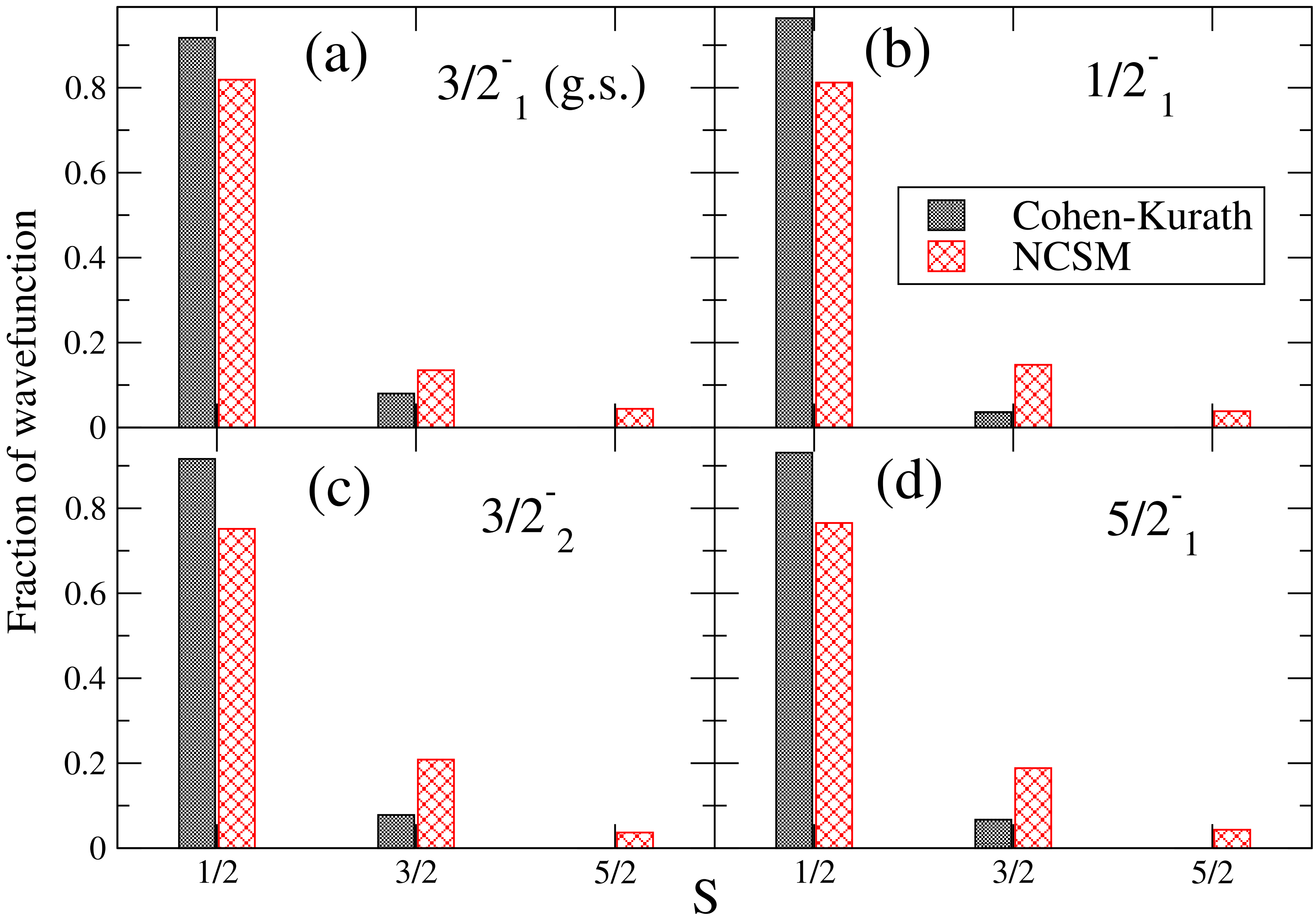
Phenomenological Cohen-Kurath *m*-scheme dimension: 62

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





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



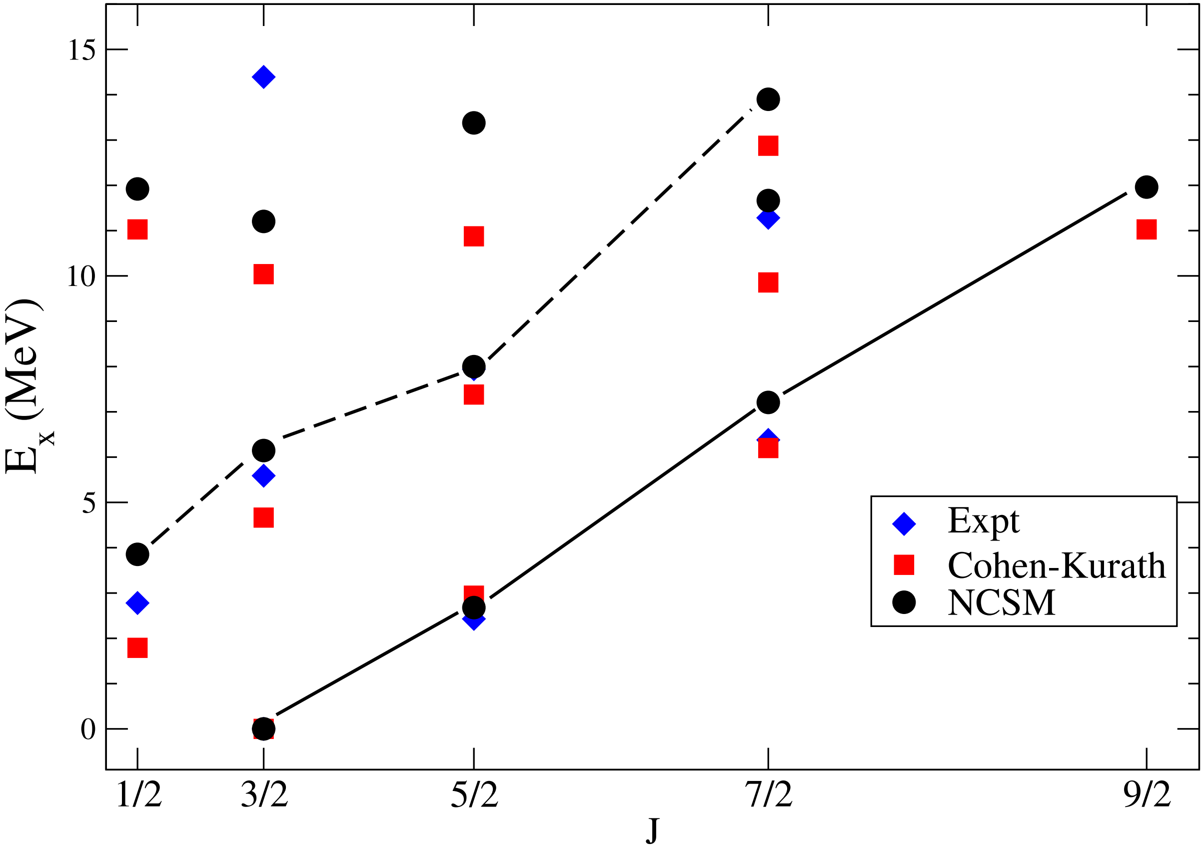
Fraction of wavefunction
0
0.2
0.4
0.6
0.8
(a)
3/2⁻₁ (g.s.)
(b)
1/2⁻₁
Cohen-Kurath
NCSM
(c)
3/2⁻₂
(d)
5/2⁻₁
1/2
3/2
5/2
S

Large Scale Shell-Model Calculations for Open-shell nuclei

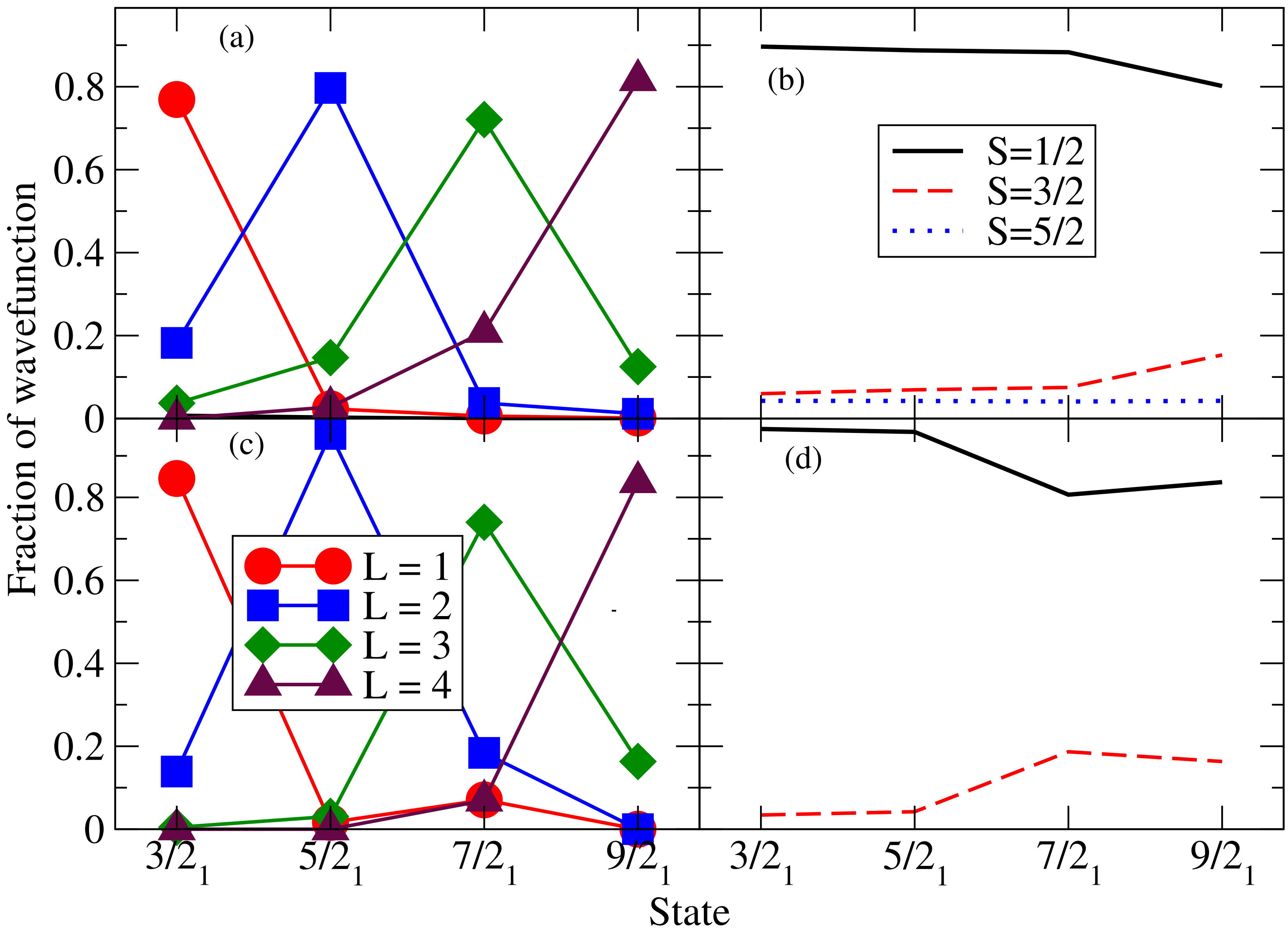
^{9}Be

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

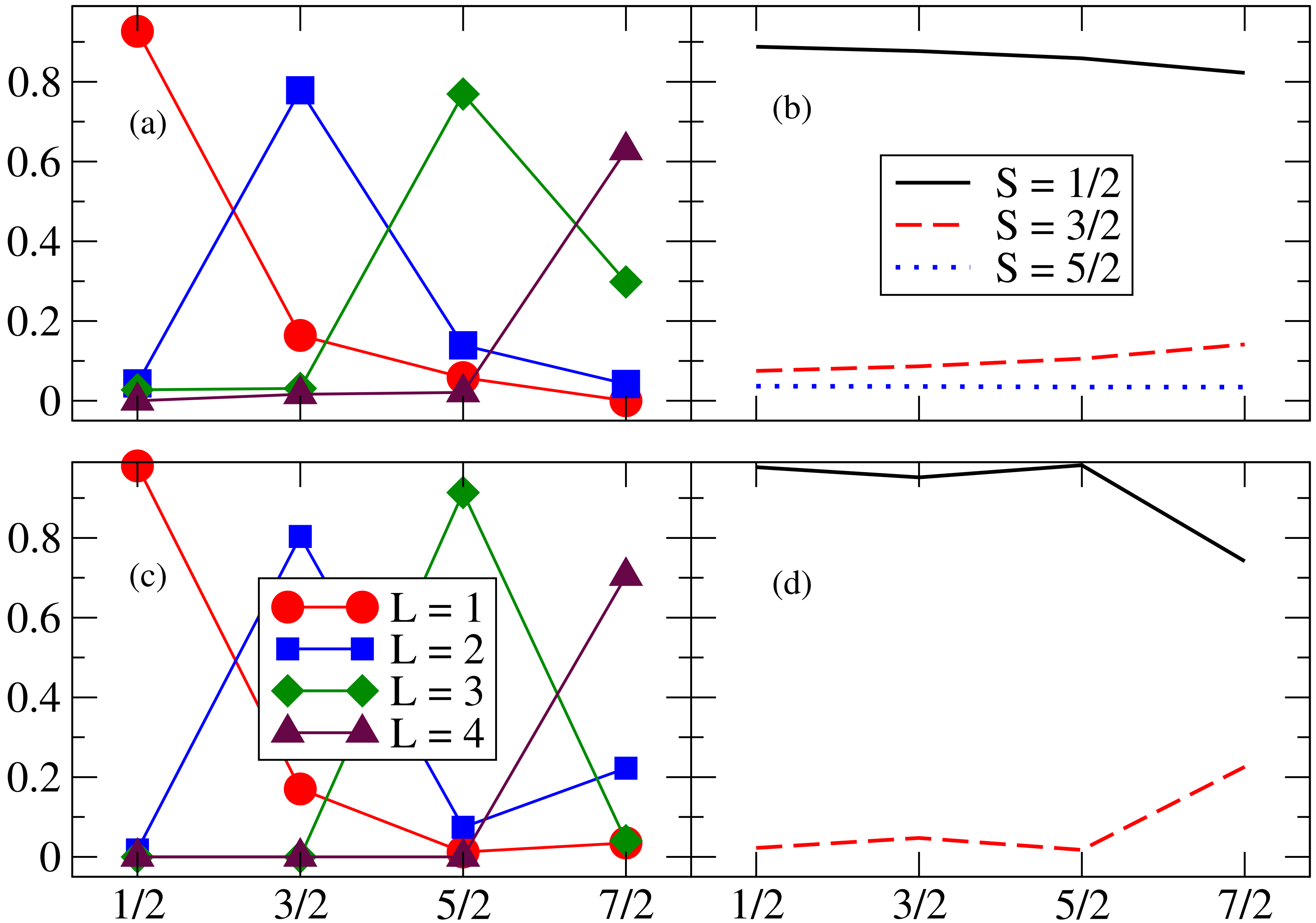
NCSM: N3LO chiral 2-body force SRG evolved to λ = 2.0 fm^{-1}, N_{max} = 6, $\hbar\omega$=22 MeV
m-scheme dimension: 5.2 million



9Be ground state band



9Be excited state band

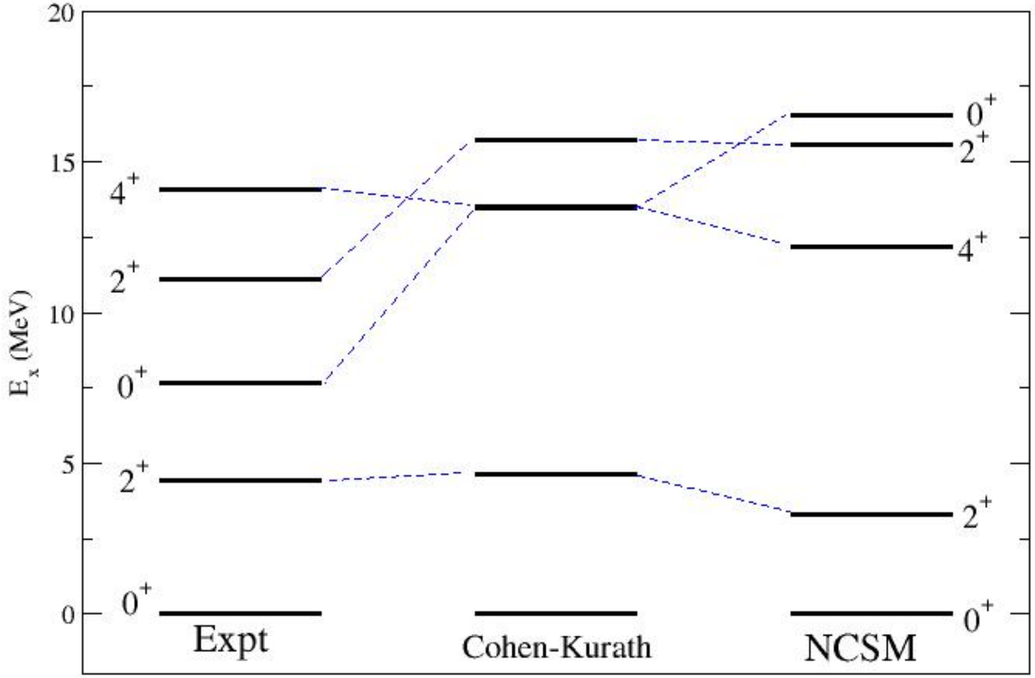


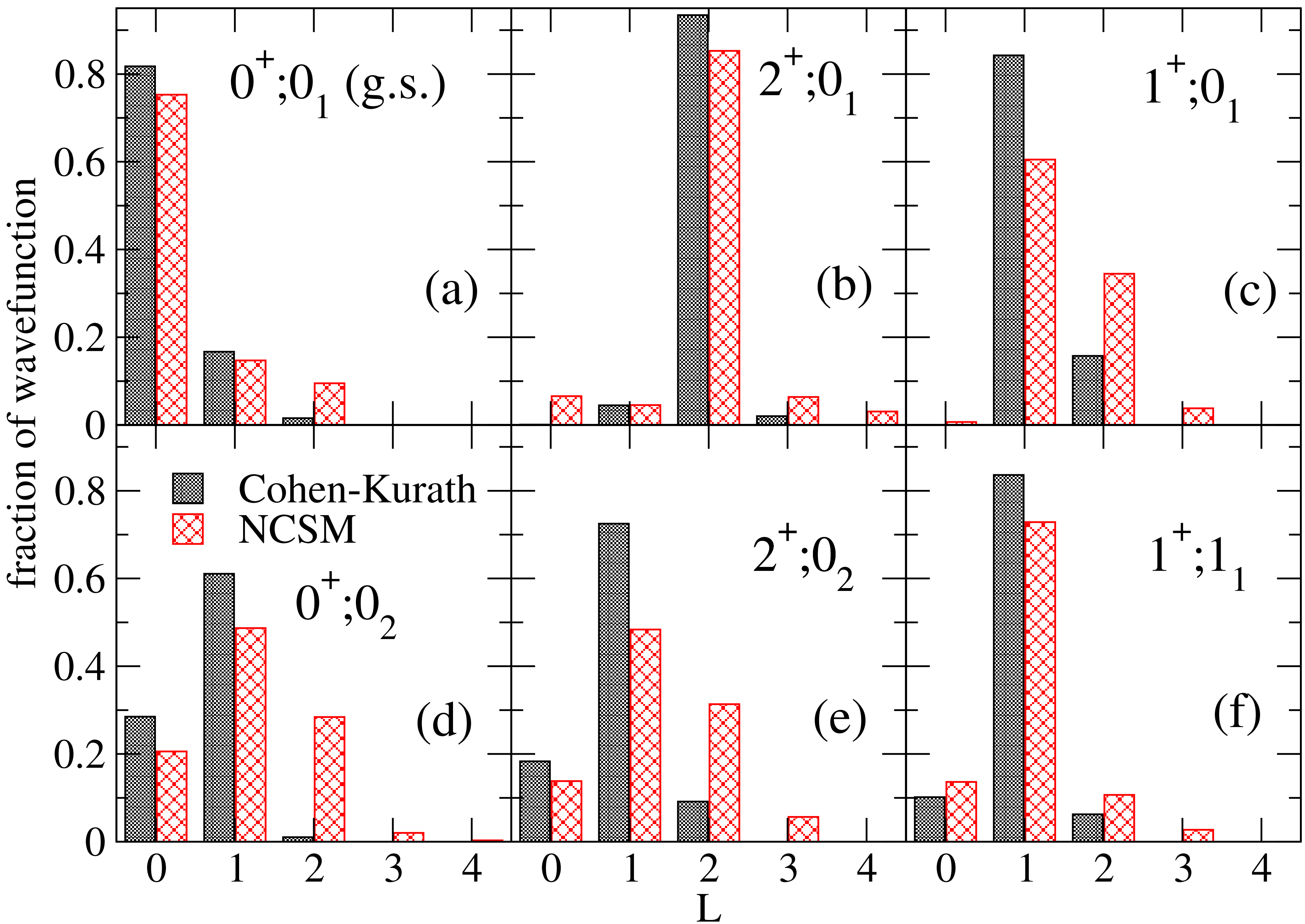
Large Scale Shell-Model Calculations for Open-shell nuclei

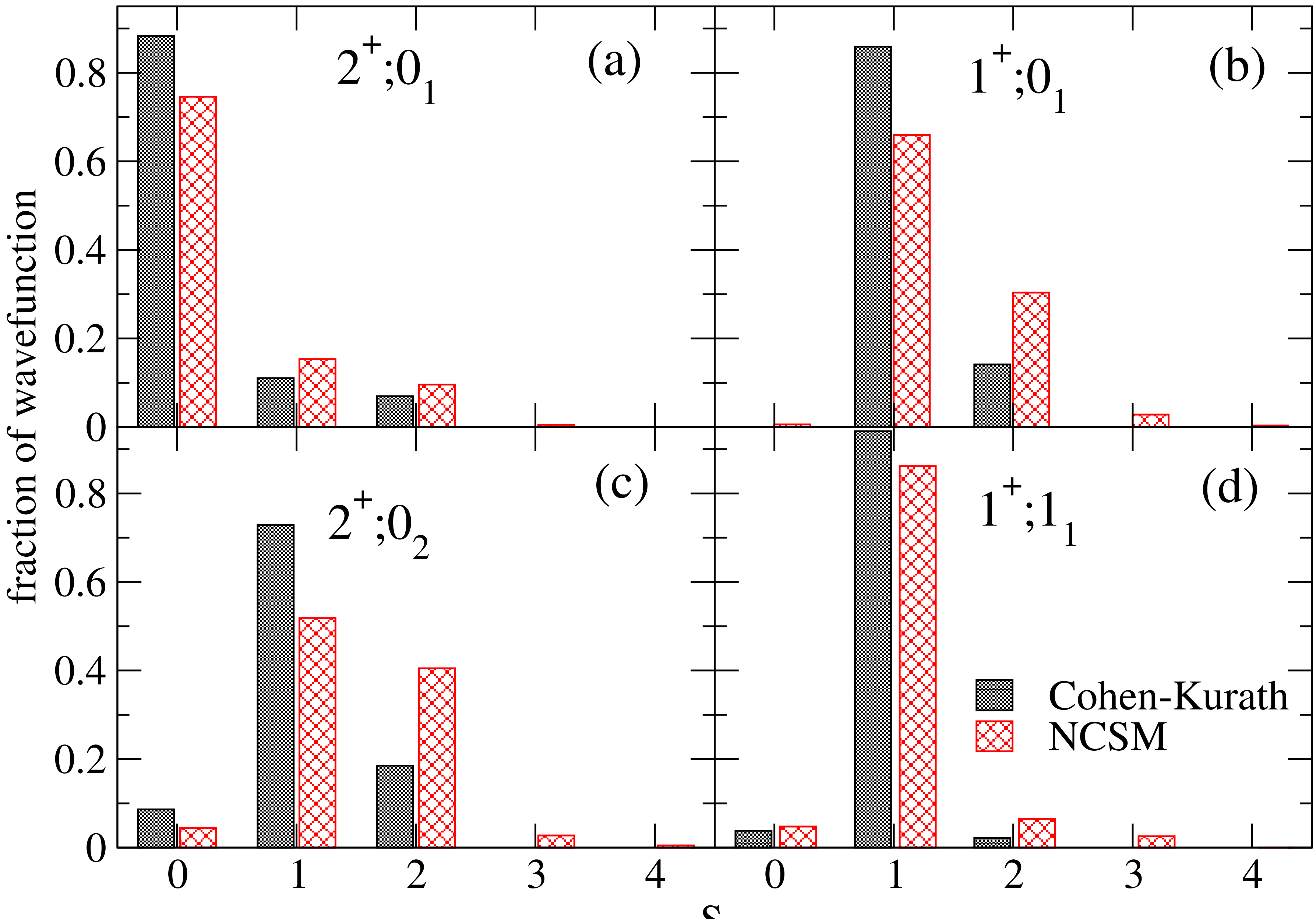
^{12}C

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




0+;01 (g.s.)
(a)
2+;01
(b)
1+;01
(c)
0+;02
(d)
2+;02
(e)
1+;11
(f)
Cohen-Kurath
NCSM
fraction of wavefunction
0
0.2
0.4
0.6
0.8
0 1 2 3 4
L



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

Summary and looking forward

We live in a dynamic universe….
can't understand it without understanding transitions!

-- We (and others) can now compute *ab initio* giant resonances
in agreement with expt
-- Some evidence for Brink hypothesis for GDRs, not so for other transitions
-- Gamow-Teller transitions are "simple" yet behavior is not trivial
(i.e., some transitions converge quickly with N_{max}, others not)
-- Some simple pictures (L-S coupling) work across vast differences in models

Summary and looking forward

But getting *calculations* = experiment is not enough!

Can we understand systematic behavior?
for example, systematics of GDRs,
Brink hypothesis

Some tools:
spectral distribution theory (moment methods) → Brink hypothesis
→ sum rules

decomposition into irreps (e.g., L-S, SU(4) irreps for Gamow-Teller)

"More work to be done!"