Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

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Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

Part I: Progress on the BIGSTICK shell model code

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

Part II: Transitions and the Brink-Axel hypothesis

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

Part III: *ab initio* Gamow-Teller transitions (in progress)

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Part I: Progress on the BIGSTICK shell model code

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

Many-fermion code: 2nd 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 200-400M+ on desktop
--has done dimension 2 billion+ on supercomputers

45 kilolines of code
Fortran 90 + MPI + OpenMP

WHY BIGSTICK?

Comparison of nonzero matrix storage with factorization

^7Li (loop over spectators)

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

What's new with BIGSTICK?

Lanczos vectors now broken up and distributed – can go to much larger model spaces (CWJ + K. McElvain, Berkeley)

Improved reorthogonalization across MPI nodes – much faster now (K. McElvain)

Next steps:

Continue pushing performance—plan to go to dim = 9 billion by summer
Improve 3-body force capabilities, will install 4-body
Beyond Lanczos—install LOBPCG or similar algorithm

Science applications: dark matter cross-sections, transition matrix elements

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

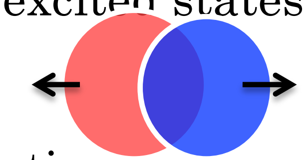
Part II: Transitions and the Brink-Axel hypothesis

+ 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

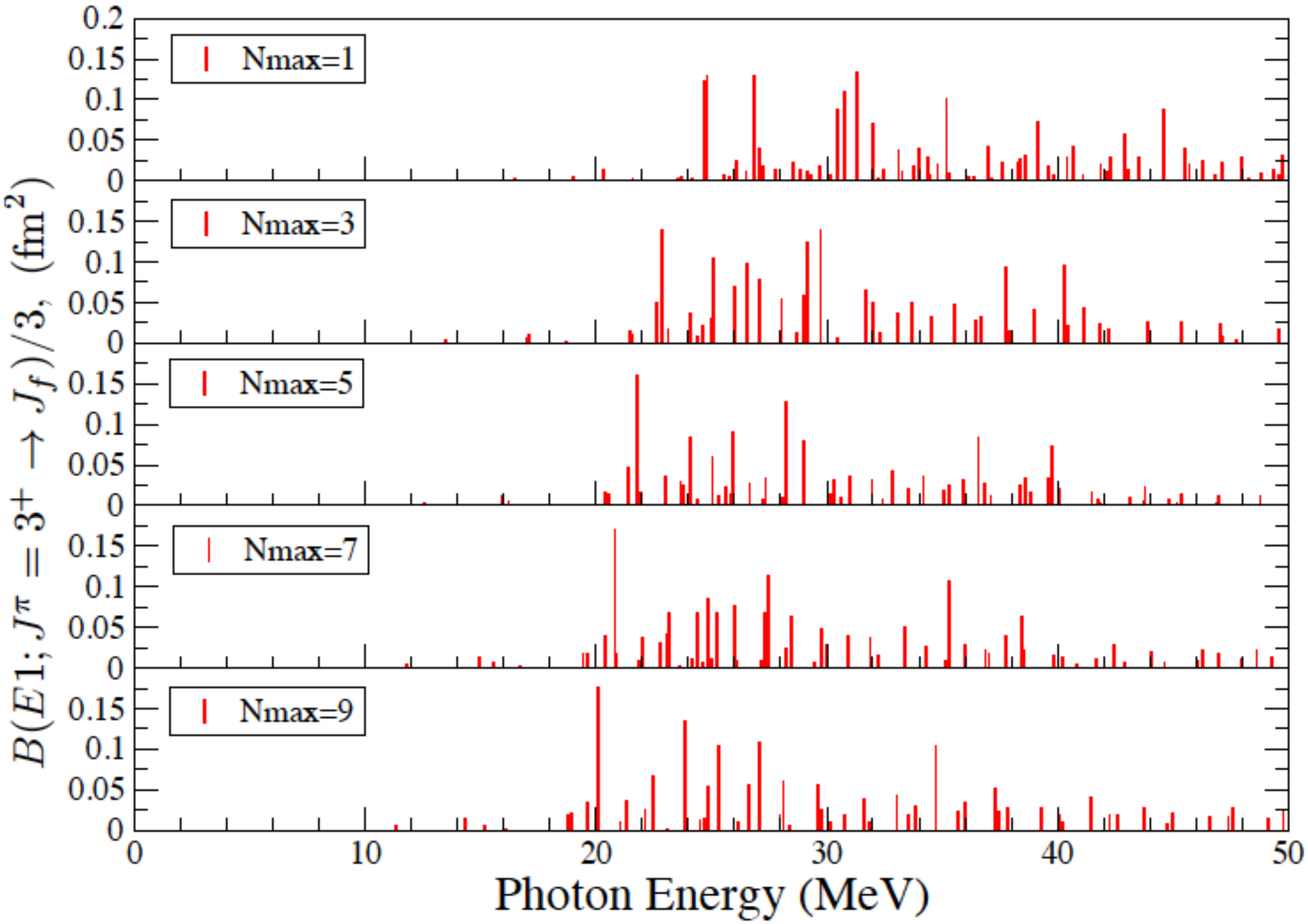
$$S(E_i, E_x) = \sum_f \left| \langle f | \hat{T} | i \rangle \right| \delta(E_x - E_f + E_i)$$

"Transition strength function"

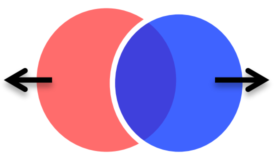
Brink-Axel: "S(E_i,E_x) independent of E_i"

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

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

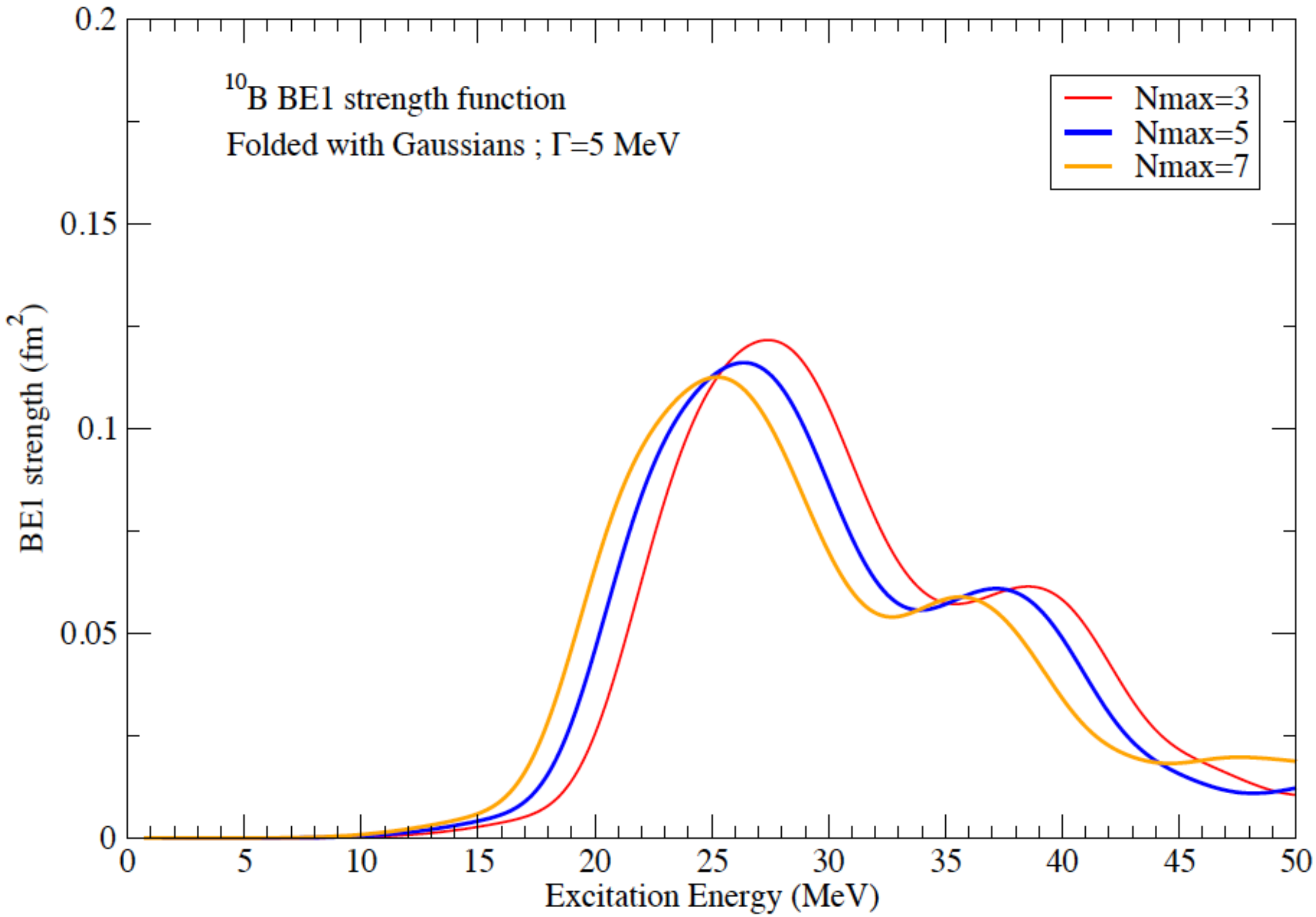


^{10}B E1 response



Electric dipole

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?

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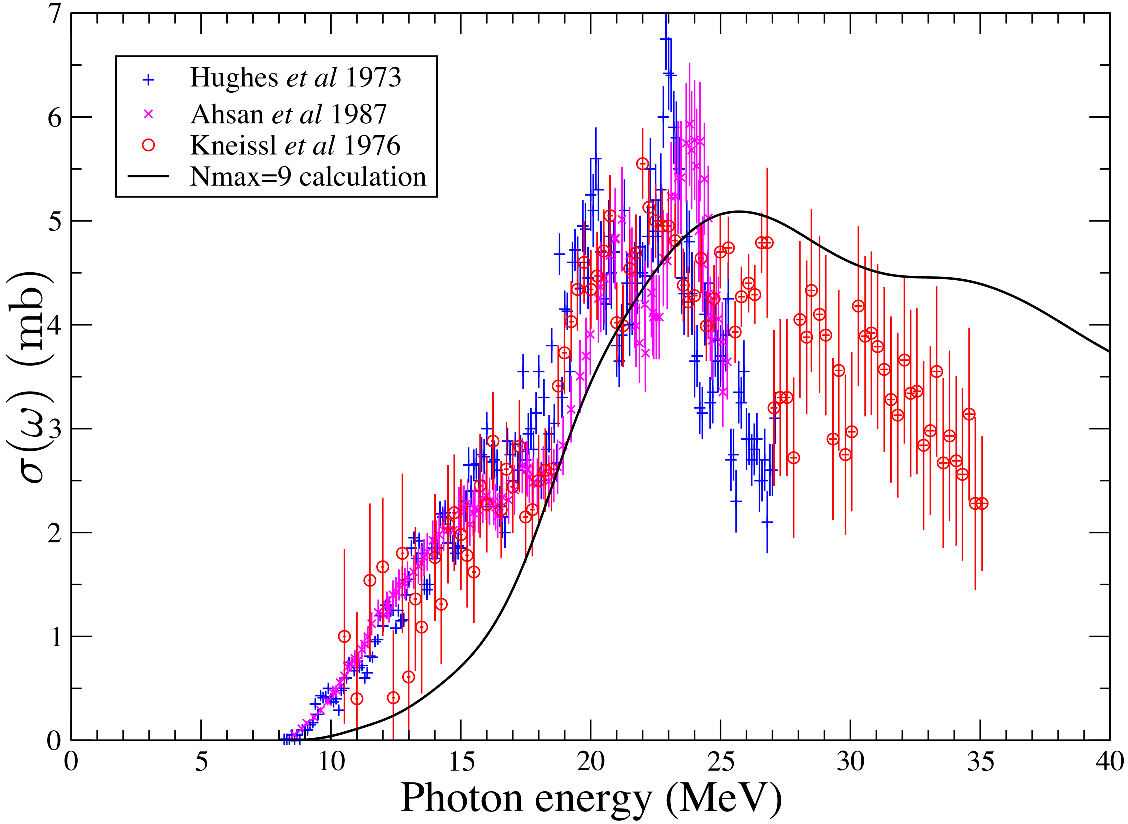

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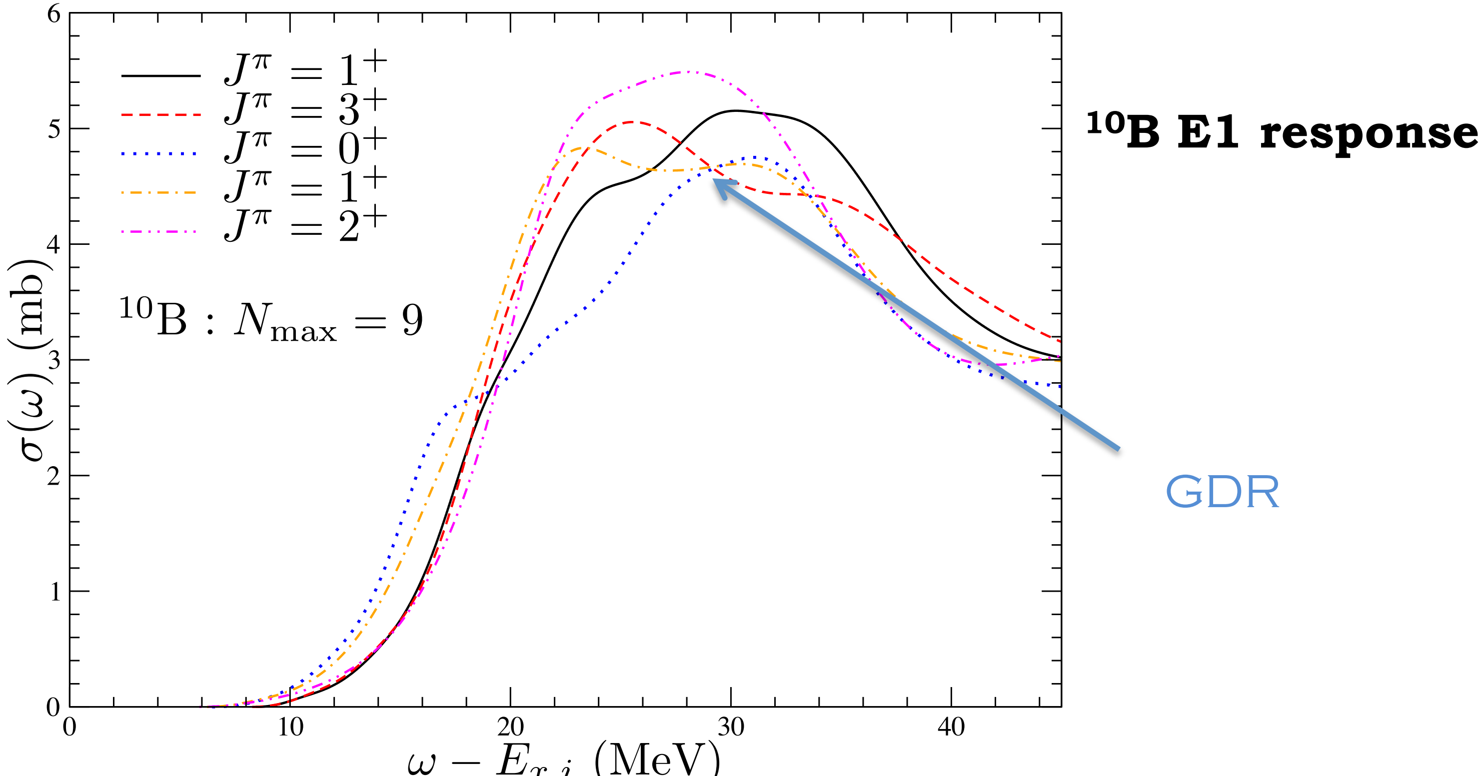


Brink-Axel: "S(E_i,E_x) independent of E_i"

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

Is this true in general? What if you look at more states?

Is this true for other operators? *

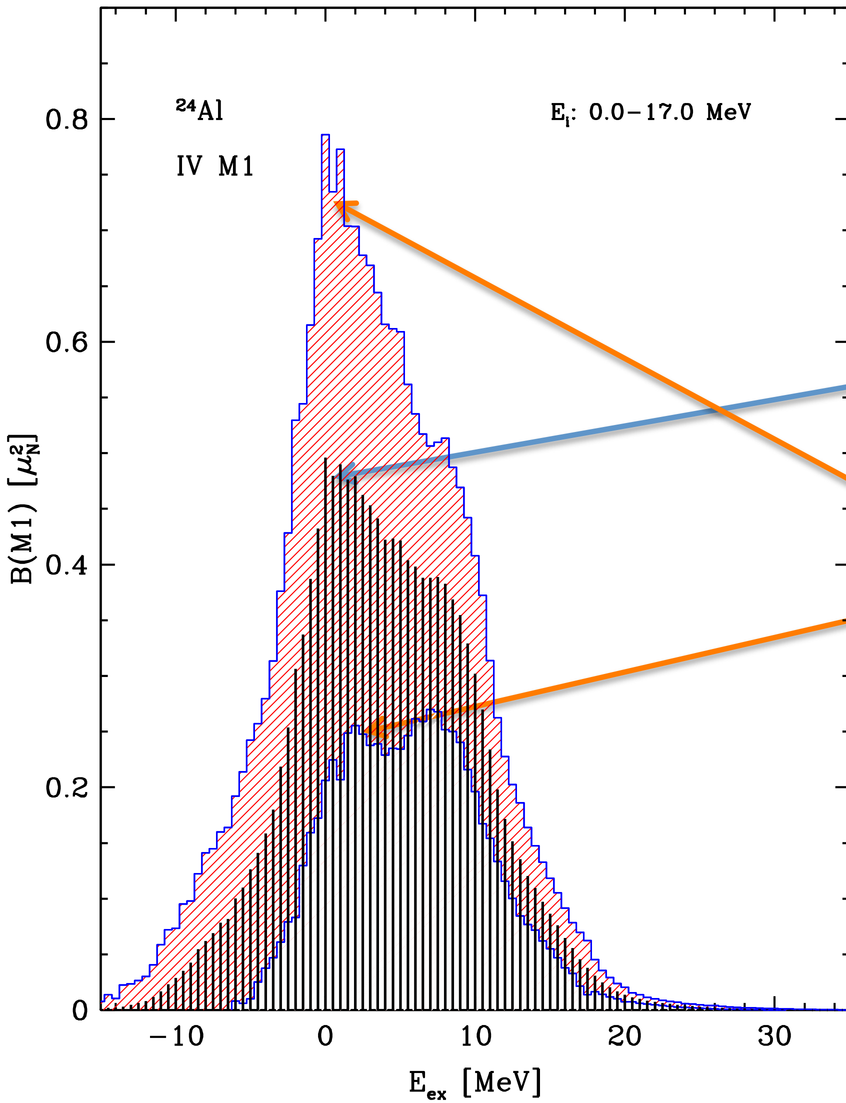
* Some evidence to the contrary (with Gamow-Teller operator): Frazier, Brown, Millener, and Zelevinsky, Phys. Lett B **414**, 7 (1997); Misch, Fuller, and Brown, PRC 90, 065808 (2014)

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 Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

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

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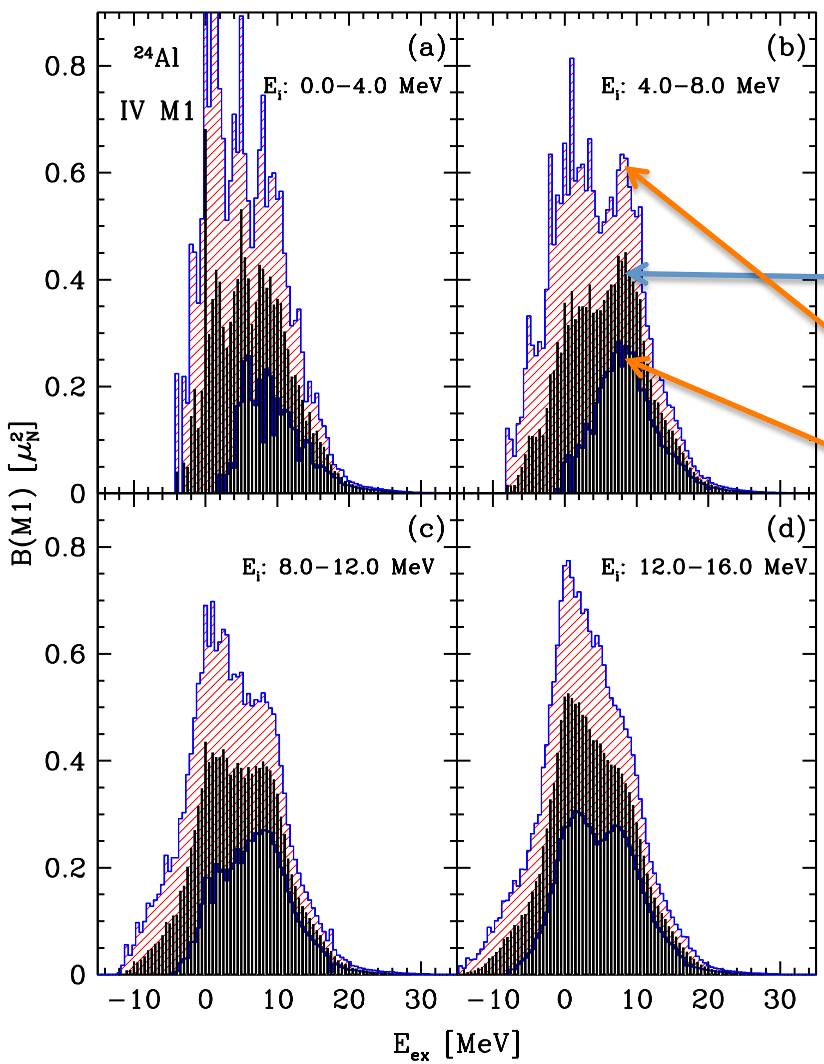
Took energy bins of initial states, computed strength functions, and computed average strength function + fluctuations about average



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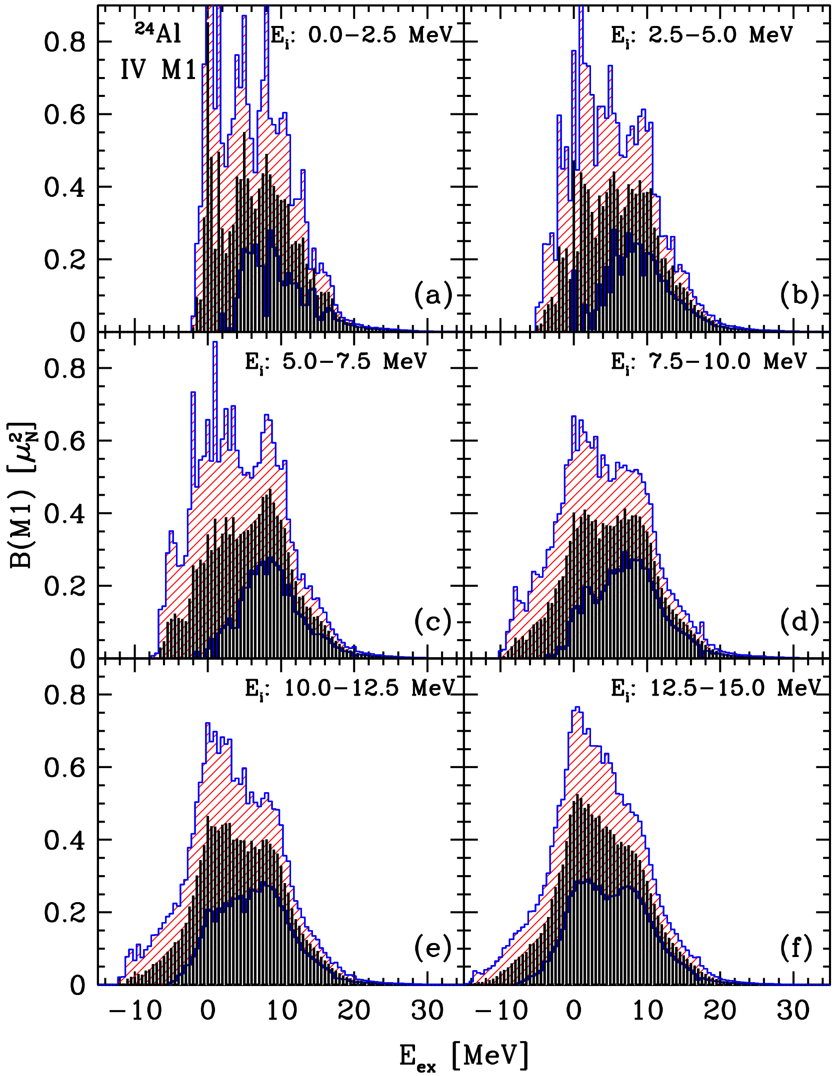
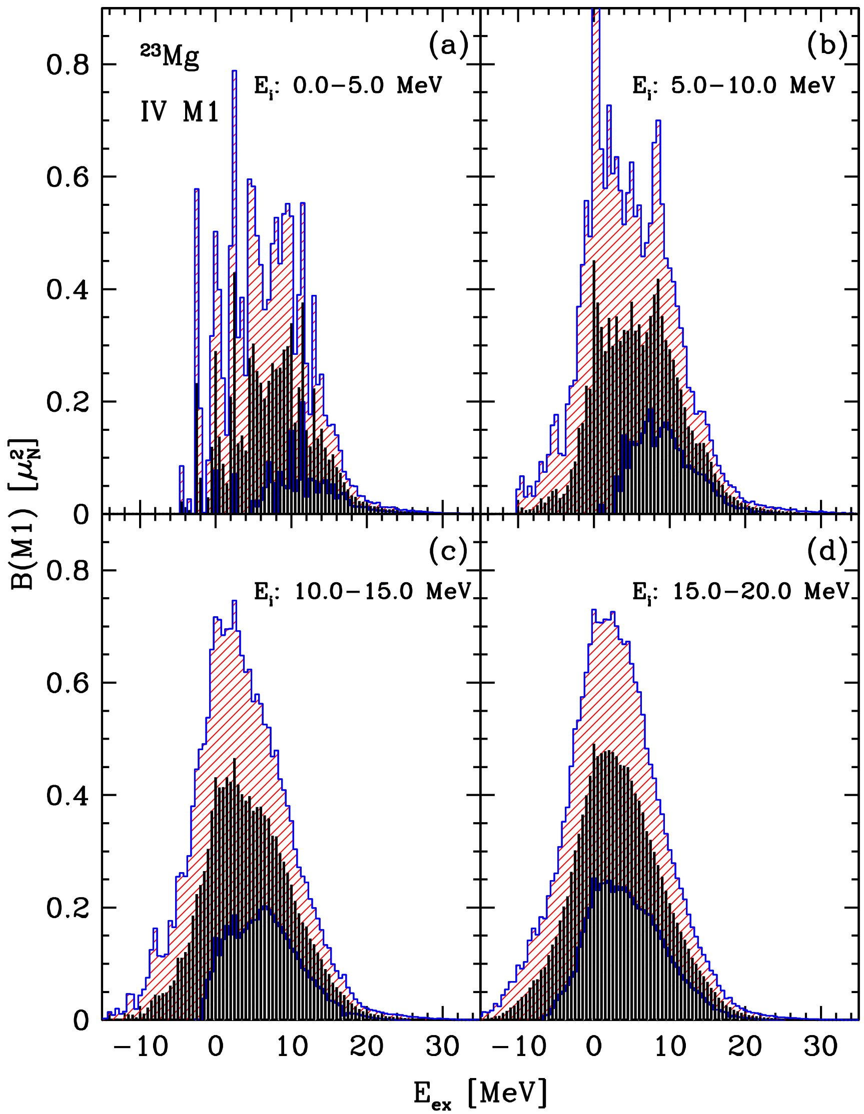


^{24}Al with isovector M1

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

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



^{23}Mg with isovector M1

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

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

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

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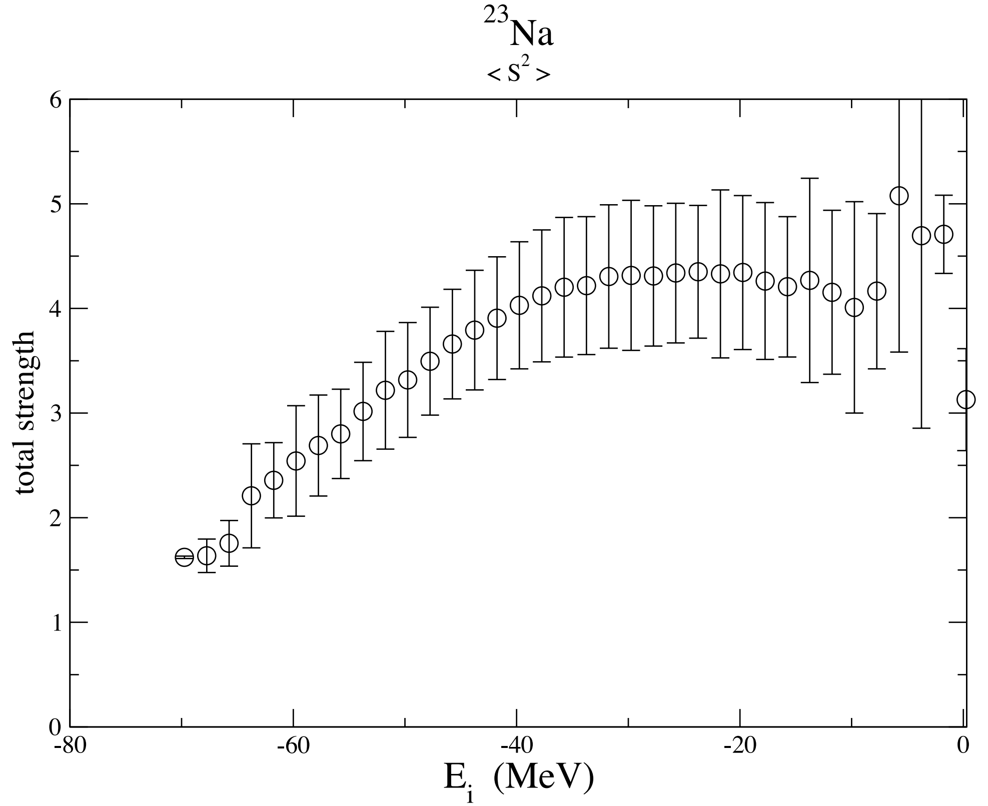
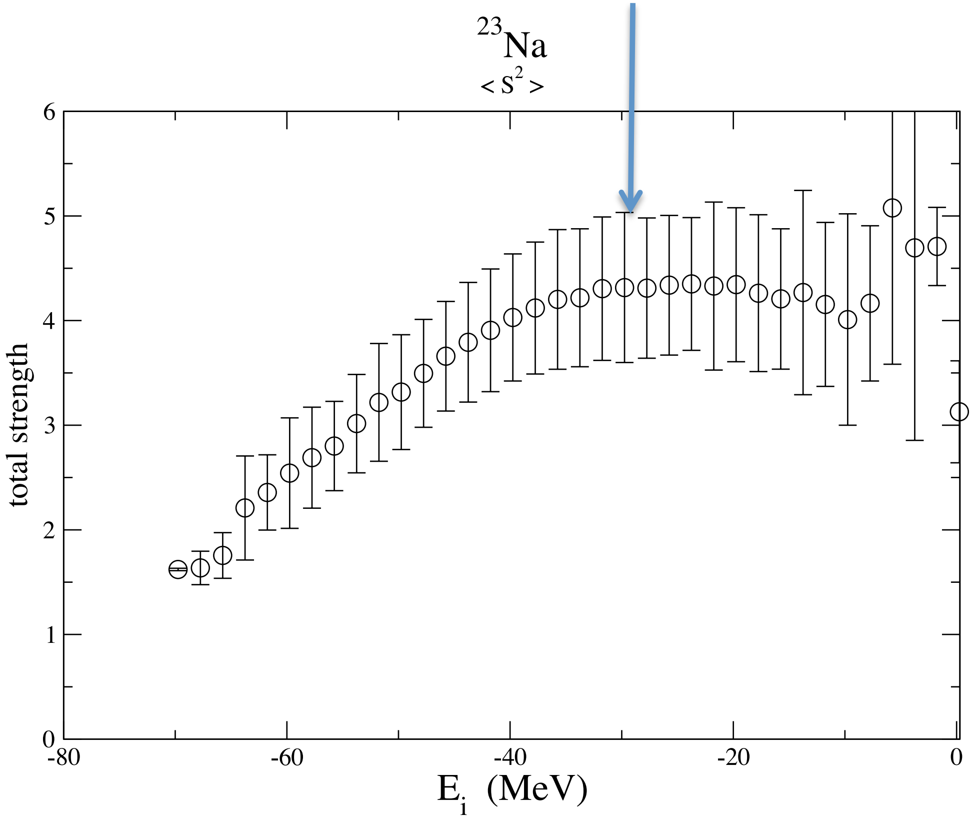
The total strength (or *non-energy-weighted sum rule*)

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



Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

$$(\Delta S_0(E_i))^2 = \left\langle i \left| \left(\hat{T}^+ T\right)^2 \right| i \right\rangle$$



The fluctuations about the average are also easy to represent

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

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!

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

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

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

Slope is given by < O H > - < O > < H >

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

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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

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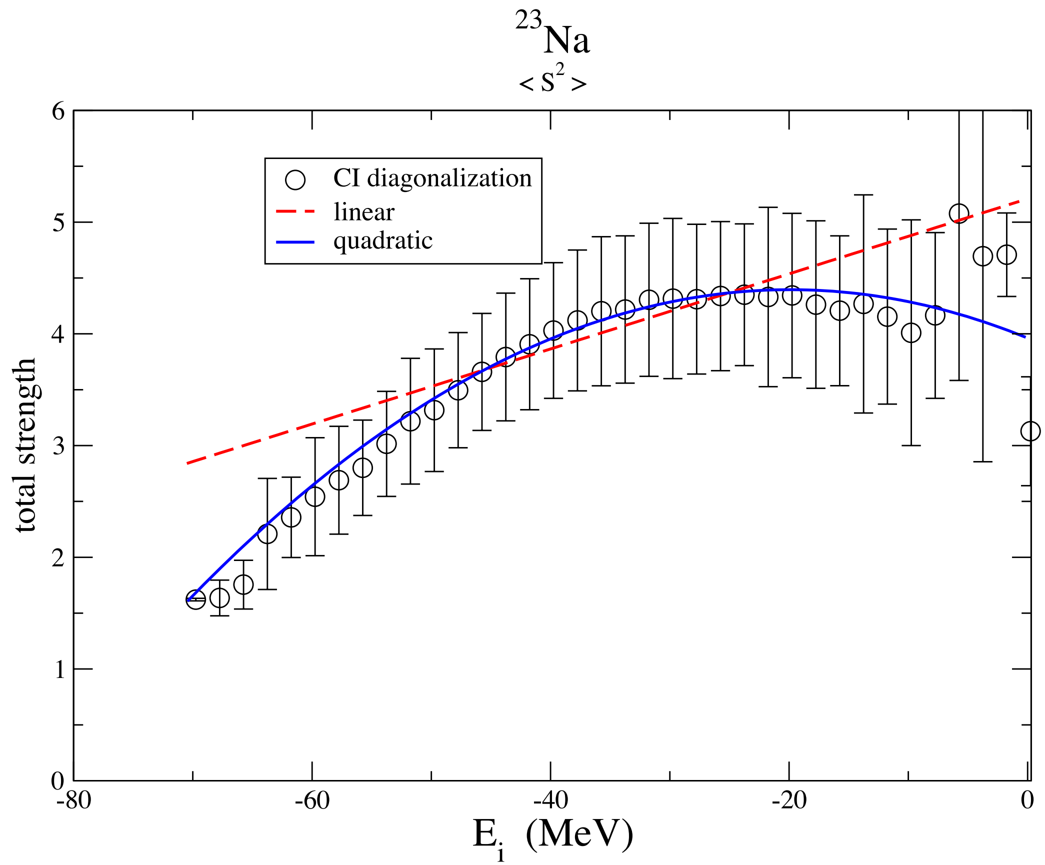

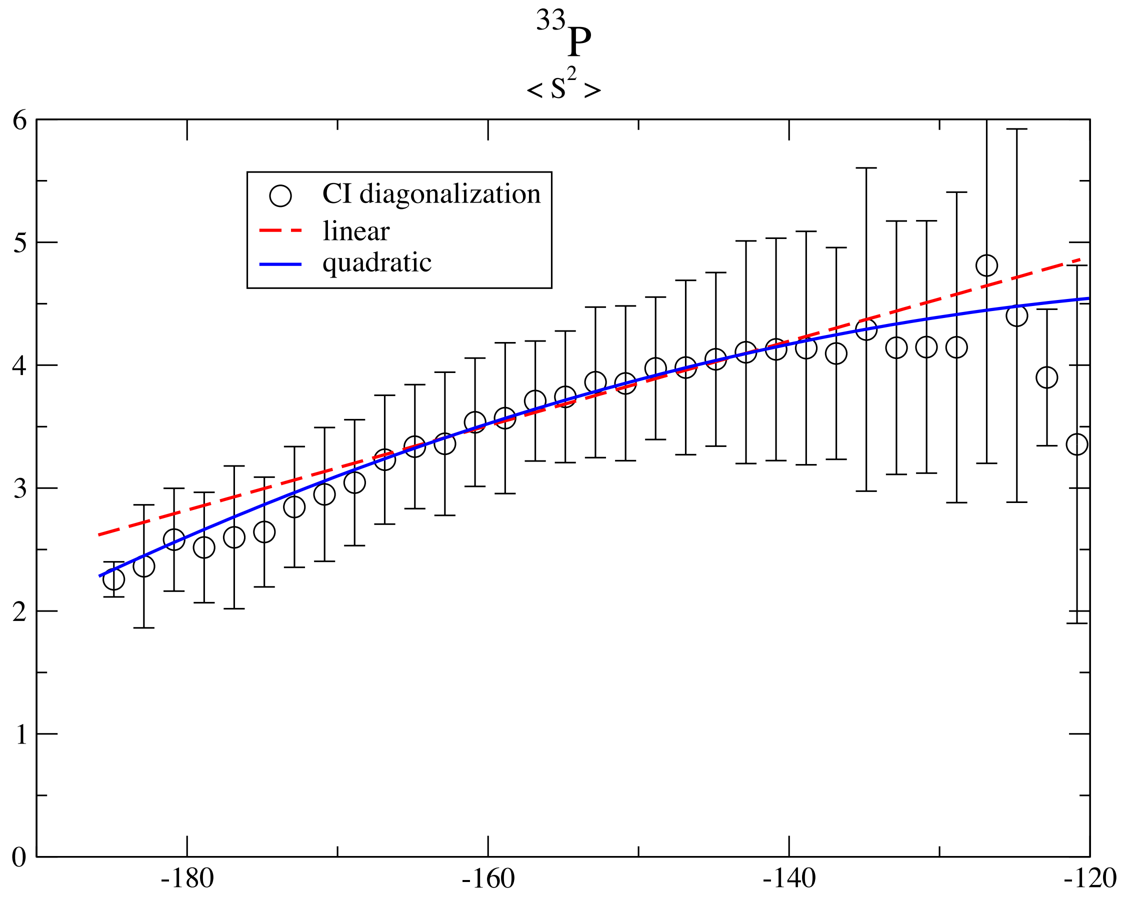

33P
< S2 >
CI diagonalization
linear
quadratic
6
5
4
3
2
1
0
-180
-160
-140
-120

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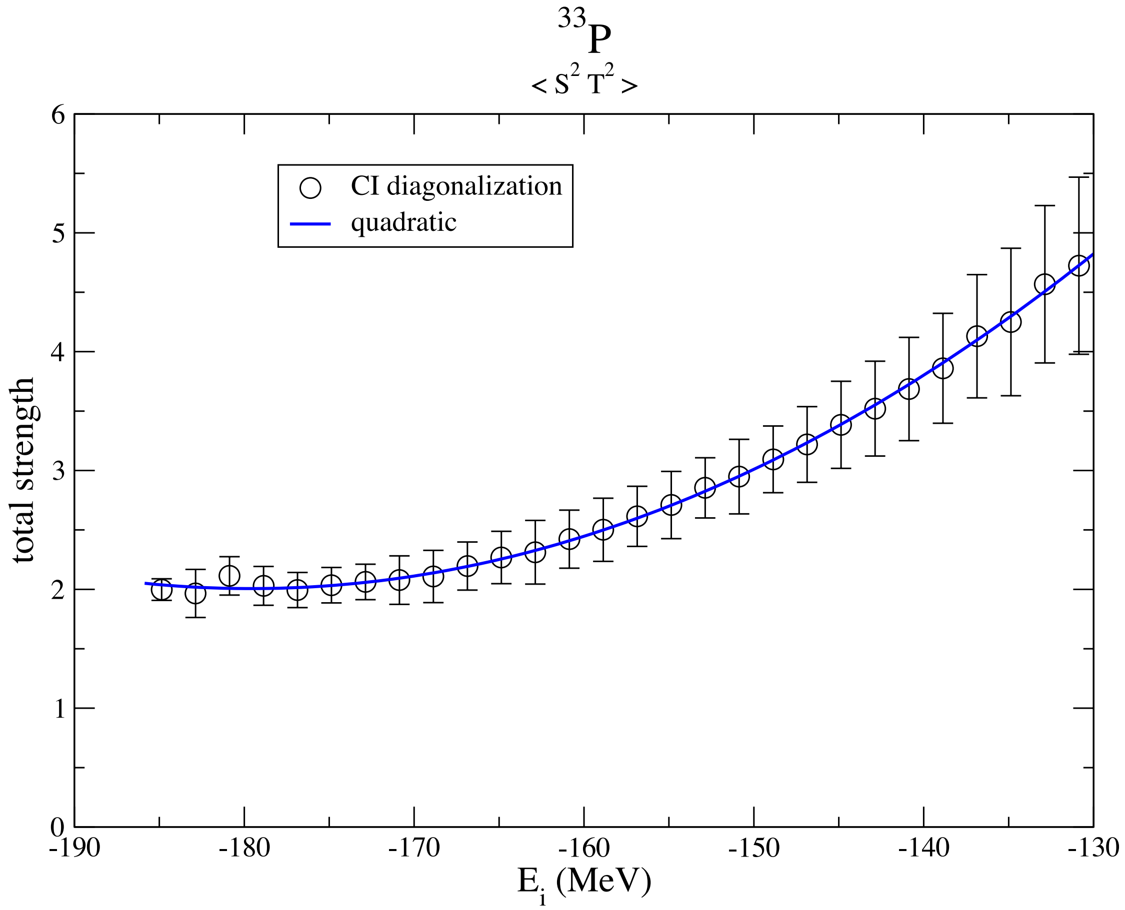

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

What we do learn from this?

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

What we do learn from this?

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

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

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

Part III: *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)

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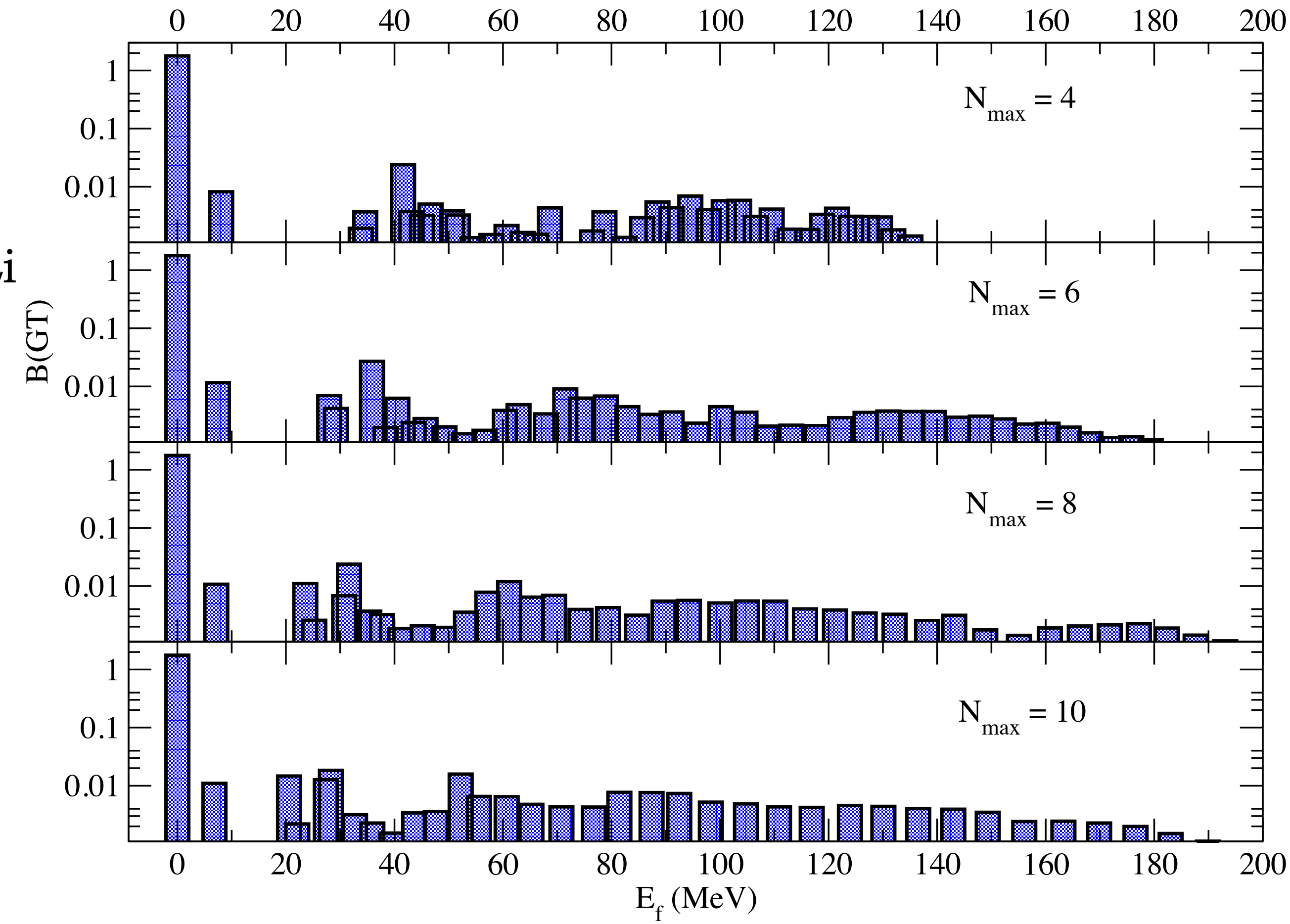
$^6He \rightarrow {}^6Li$

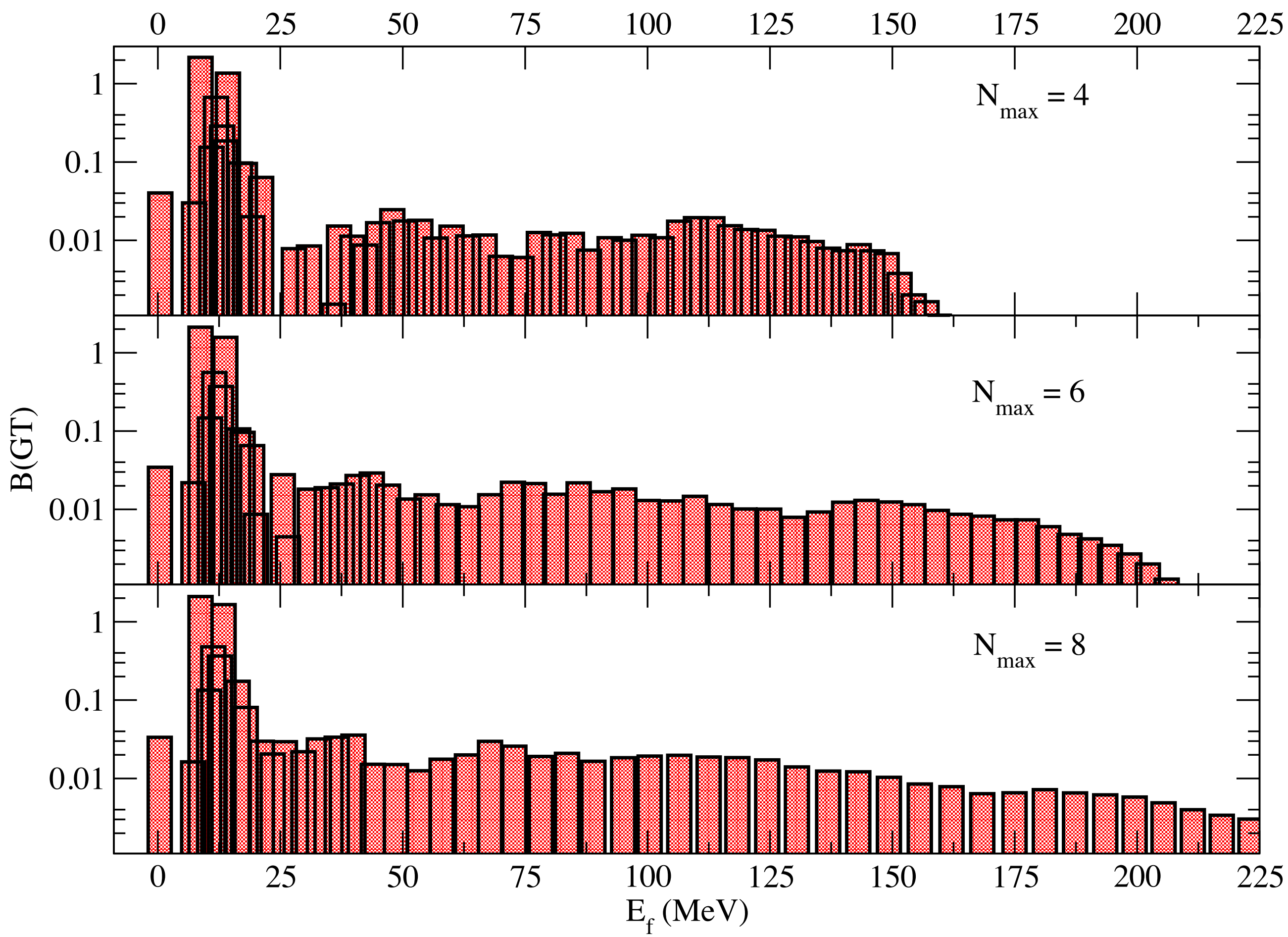


Preliminary!

Chiral 2-body forces SRG evolved to $\lambda=2\ fm^{-1}$)

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

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

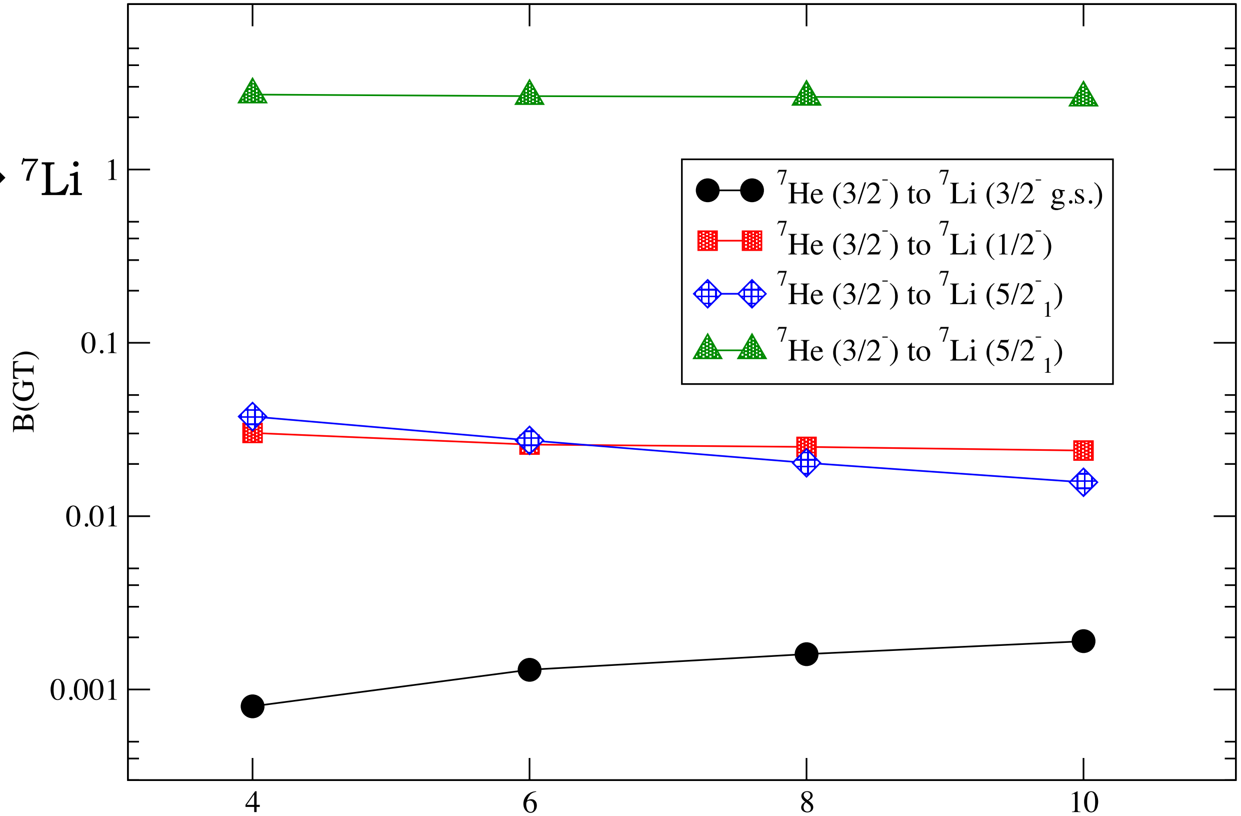


Preliminary!

(Run on desktop machine with BIGSTICK)

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

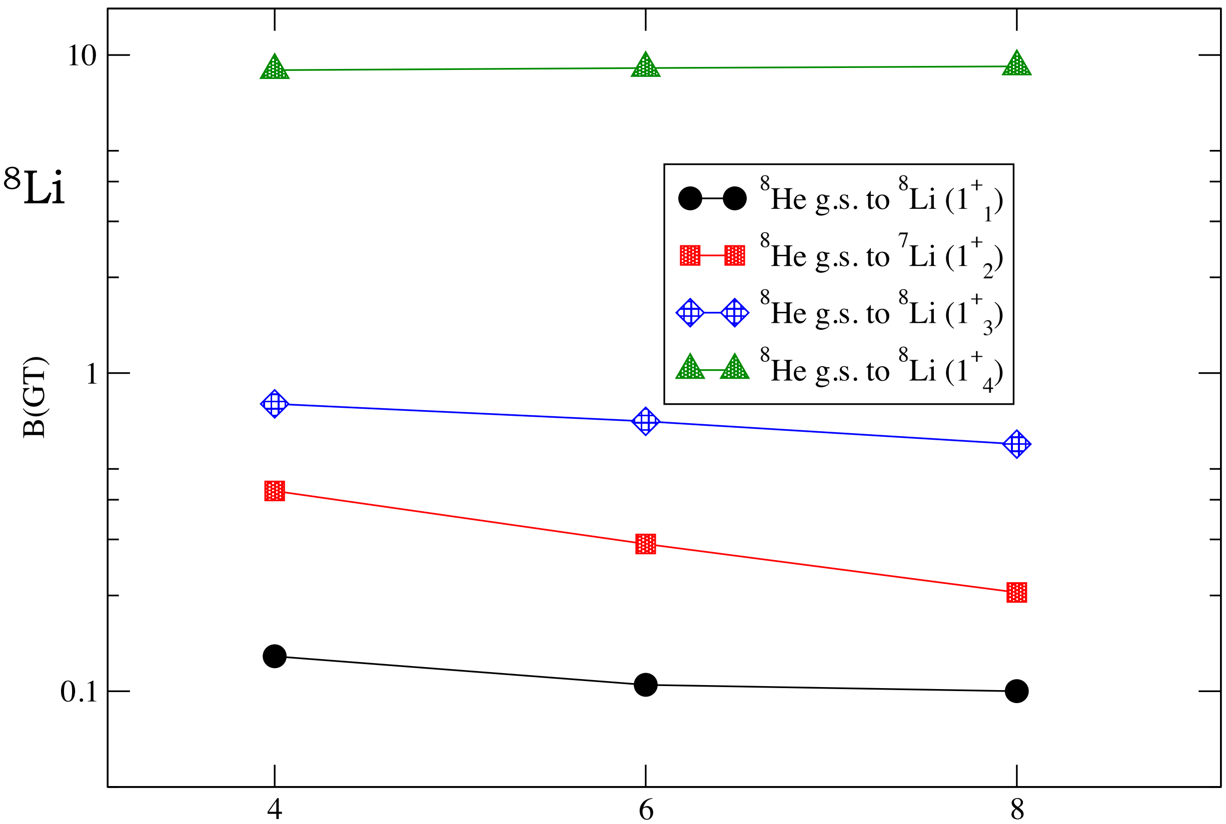
$^{7}He \rightarrow {}^{7}Li$



Preliminary!

Large Scale Calculations of Nuclear Structure and Nuclear Transition Matrix Elements

^{8}He ➔ ^{8}Li



Preliminary!

Part III: *ab initio* Gamow-Teller transitions

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…

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)

As the *ab initio* community moves forward, we collectively are developing
-- "consistently evolved" operators (e.g., Micah Schuster's poster)
-- EFT-derived exchange current corrections (e.g. R. Wiringa, S. Pastore)

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., SU(4) irreps for Gamow-Teller)

"More work to be done!"