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Transition strengths and sum rules in the no-core shell model

Calvin W. Johnson

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

"This research used resources (ERCAP award) of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231."

TRIUMF Workshop on *ab initio* stuff 2018

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The BIGSTICK shell-model code is released!

Download from:
github.com/cwjsdsu/BigstickPublick

Manual at arXiv:1801.08432

Links to BIGSTICK and other free, open-source many-body codes available through

fribtheoryalliance.org

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The BIGSTICK shell-model code is released!

BIGSTICK uses a simple M-scheme (fixed J_z) basis of occupation-representation Slater determinants.

It solves the many-body matrix eigenvalue problem $\mathbf{H}\ |\psi> = E\ |\psi>$ by the Lanczos algorithm

$$\mathbf{H}\ |v_1> = \alpha_1\ |\ v_1> + \beta_1\ |v_2>$$
$$\mathbf{H}\ |v_2> = \beta_1\ |v_1> + \alpha_2\ |v_2> + \beta_2\ |v_3>$$
$$\mathbf{H}\ |v_3> = \beta_2\ |v_2> + \alpha_3\ |v_3> + \beta_3\ |v_4>$$

etc.

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The BIGSTICK shell-model code is released!

BIGSTICK uses Lanczos for a number of applications, as well see.

The Hamiltonian matrix elements are ``factorized'' and reconstructed on-the-fly. See CWJ, Ormand, and Krastev, Comp. Phys. Comm. **184**, 2761 (2013)

Has both OpenMP and MPI parallelization;
Runs on laptops up through supercomputers.
Both phenomenological and no-core shell model spaces and interactions.

Transitions

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In particular β and γ transitions tell us a lot about nuclear structure.

-- Individual transition strengths
-- Transition strength functions
-- Transition strength sum rules

-- An important and controversial question is the validity of the *Brink-Axel hypothesis:* that strength functions off excited states look "just like" ground state strength functions

The Lanczos trick for strength functions

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(See also talk by Nir Nevo Dinur on Wednesday)

Whitehead and Watt *J Phys G* **4**, 835(1978)
Whitehead, Watt, and Kelvin. *Phys Lett* ***B*** **89**, 313 (1980)
Whitehead in *Theory and Applications of Moment Methods in Many-Fermion Systems*, 235 (1980)
Bloom, Prog. Part. Nucl. Phys **11**, 205 (1984)

Strength function

$$S(E_x) = \sum_f \delta(E_f - E_i - E_x) \left| \langle f | \hat{O} | i \rangle \right|^2$$

The Lanczos trick for strength functions

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Strength function

$$S(E_x) = \sum_f \delta(E_f - E_i - E_x) \left| \langle f | \hat{O} | i \rangle \right|^2$$

Lanczos trick:

* Generate some initial state (e.g. the g.s.)
* Let Lanczos pivot (starting vector) be

$$|v_1\rangle = \hat{O}|i\rangle$$

* Now run ordinary Lanczos iterations

The Lanczos trick for strength functions

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* Now run ordinary Lanczos iterations

$$\mathbf{H}\ |v_1\rangle = \alpha_1\ |\ v_1\rangle + \beta_1\ |v_2\rangle$$
$$\mathbf{H}\ |v_2\rangle = \beta_1\ |v_1\rangle + \alpha_2\ |v_2\rangle + \beta_2\ |v_3\rangle$$
$$\mathbf{H}\ |v_3\rangle = \beta_2\ |v_2\rangle + \alpha_3\ |v_3\rangle + \beta_3\ |v_4\rangle$$

etc.

The Lanczos trick for strength functions

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Lanczos trick, cont'd:

Diagonalize the tridiagonal Hamiltonian in the truncated Lanczos (Krylov space) basis, to get eigenstates:

$$|\psi_f> = c_{f1} |v_1> + c_{f2} | v_2> + c_{f3} | v_3> \ldots.$$

The Lanczos trick for strength functions

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Lanczos trick, cont'd:

Diagonalize the tridiagonal Hamiltonian in the truncated Lanczos (Krylov space) basis, to get eigenstates:

$$|\psi_f> = c_{f1}\,|v_1> + c_{f2}\,|\,v_2> + c_{f3}\,|\,v_3> \ldots.$$

The probability $|\,c_{f1}\,|^2 = |<\psi_f\,|v_1>|^2$

$$= \left|\langle f|\hat{O}|i\rangle\right|^2$$

that is, we can read the strength *directly* from the Lanczos process!

The Lanczos trick for strength functions

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Lanczos trick, cont'd:

This can also be used to decompose states into group irreps

Gueorguiev, Draayer, and CWJ, Phys. Rev. C **63** 014318 (2000)
CWJ, Phys. Rev. C **91**, 034313 (2015)

and project out states with good quantum numbers

CWJ, Ormand, McElvain, and Shan, arXiv:1801:08432

The Lanczos trick for strength functions

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Lanczos trick, some technical details:

We want the B-value, related to reduced matrix element:

$$B(\hat{O}) = \frac{1}{2J_i + 1} \left| \langle f || \hat{O} || i \rangle \right|^2$$

If one works in the M-scheme (fixed J_z), one must treat angular momentum carefully.

If M=0 and $J_i = 0$, then easy: multiply by $2J_f+1=2K+1$,
K = rank of operator.

If $J_i \neq 0$, then must project out states of good J_f (using Lanczos trick again) and combine with Clebsch-Gordans.
(See `BIGSTICK` manual, arxiv: 1801.08432)

The Lanczos trick for strength functions

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(Technical aside:

B-value is *average over initial states* and *sum over final states*

The Lanczos trick for strength functions

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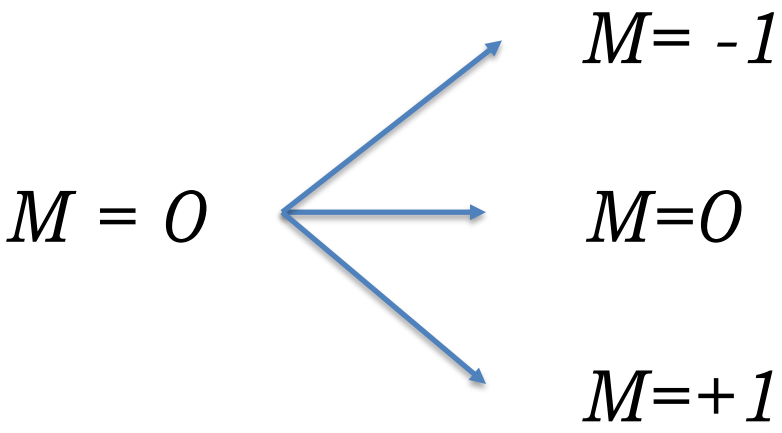
(Technical aside:

B-value is *average over initial states* and *sum over final states*

e.g. E1



The Lanczos trick for strength functions

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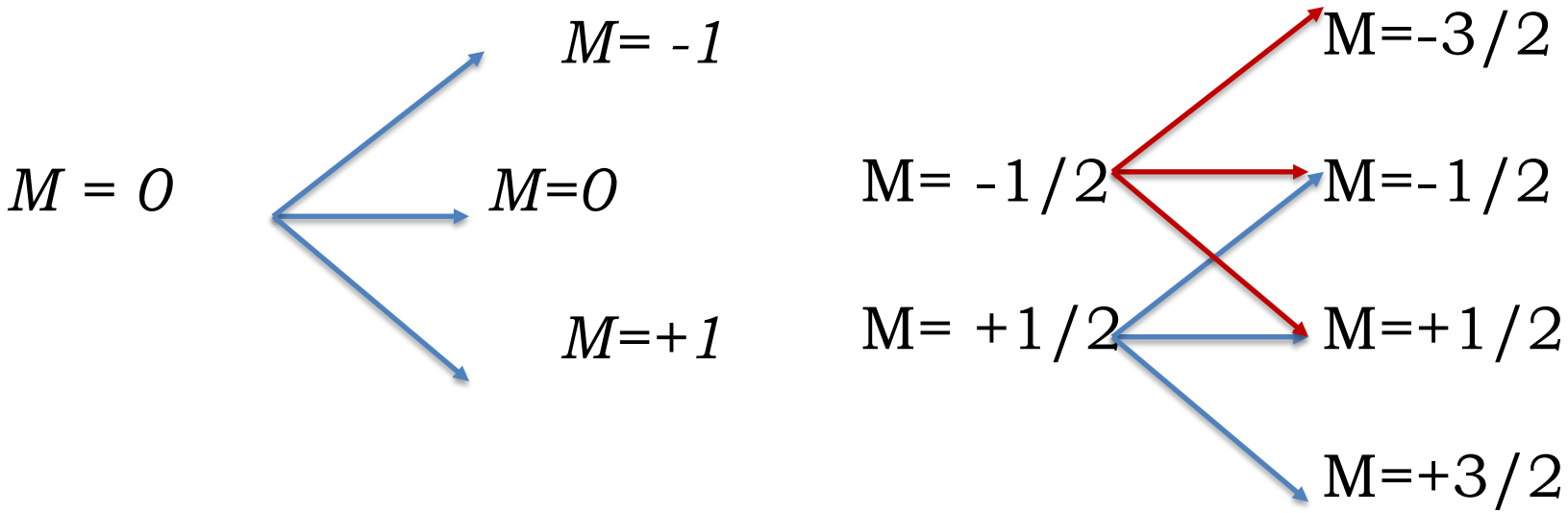

The Lanczos trick for strength functions

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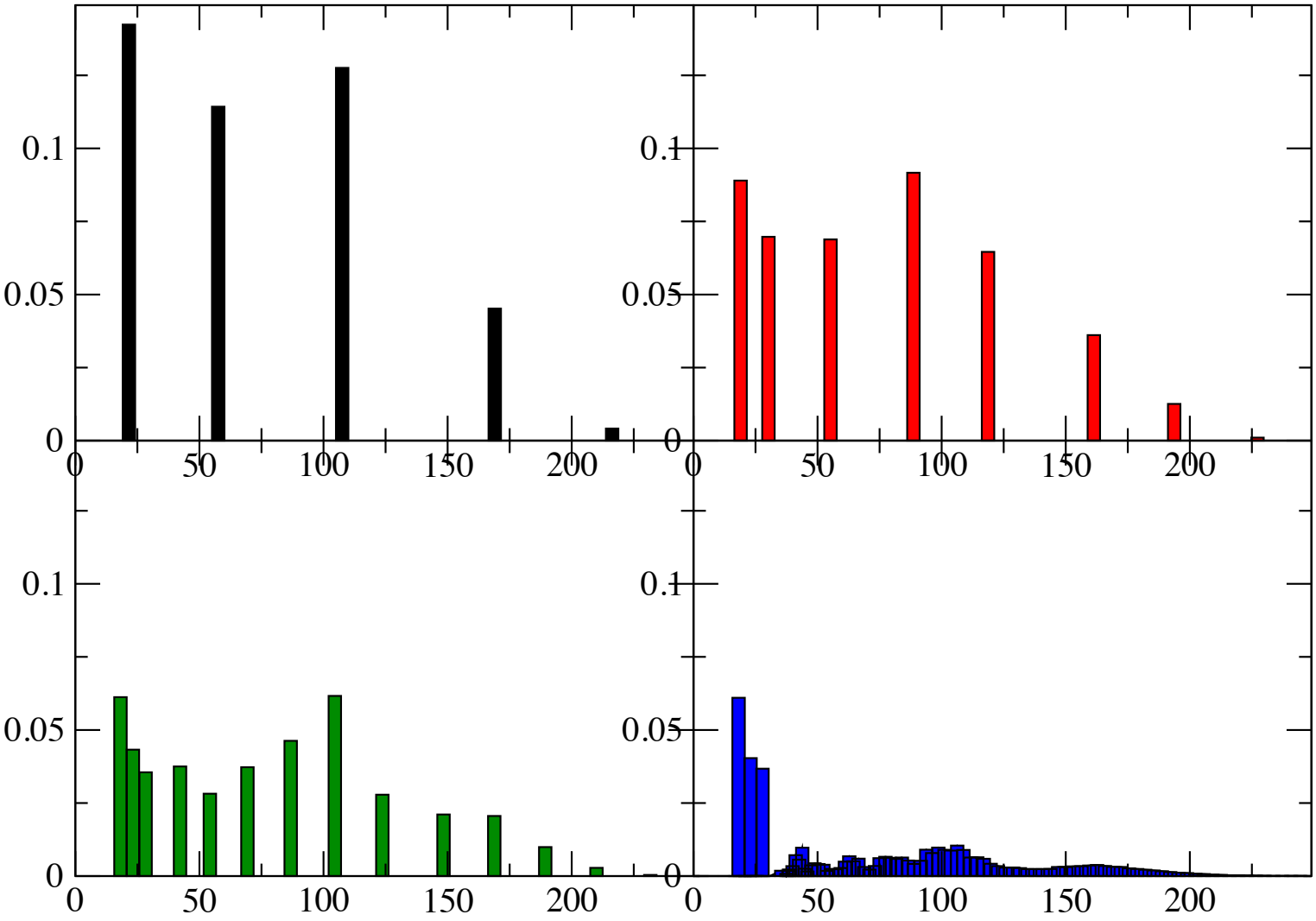
Another issue: Lanczos is an iterative scheme, and the strength function depends upon the number of iterations.

8Be. Nmax=6. Gamow-Teller



The Lanczos trick for strength functions

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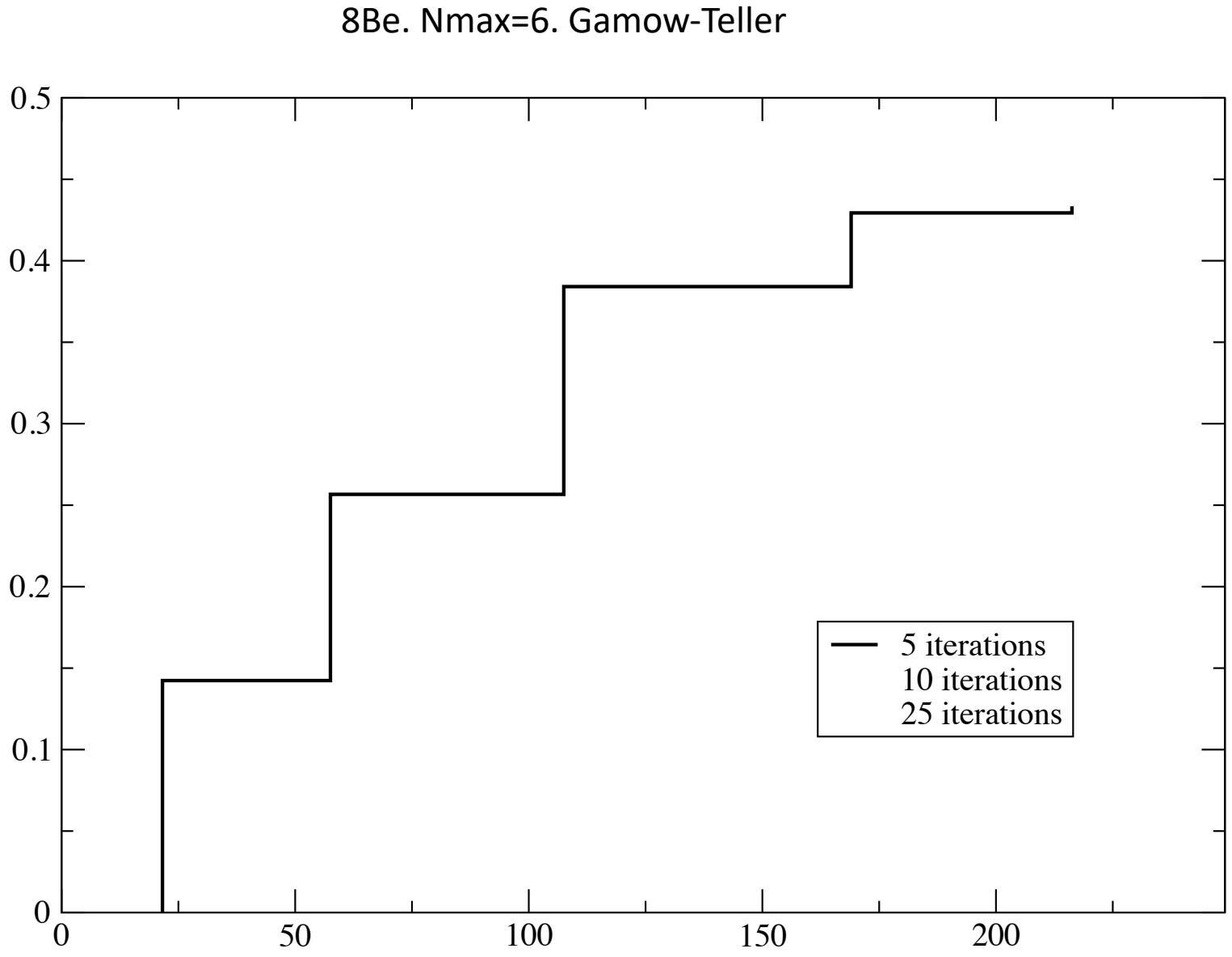
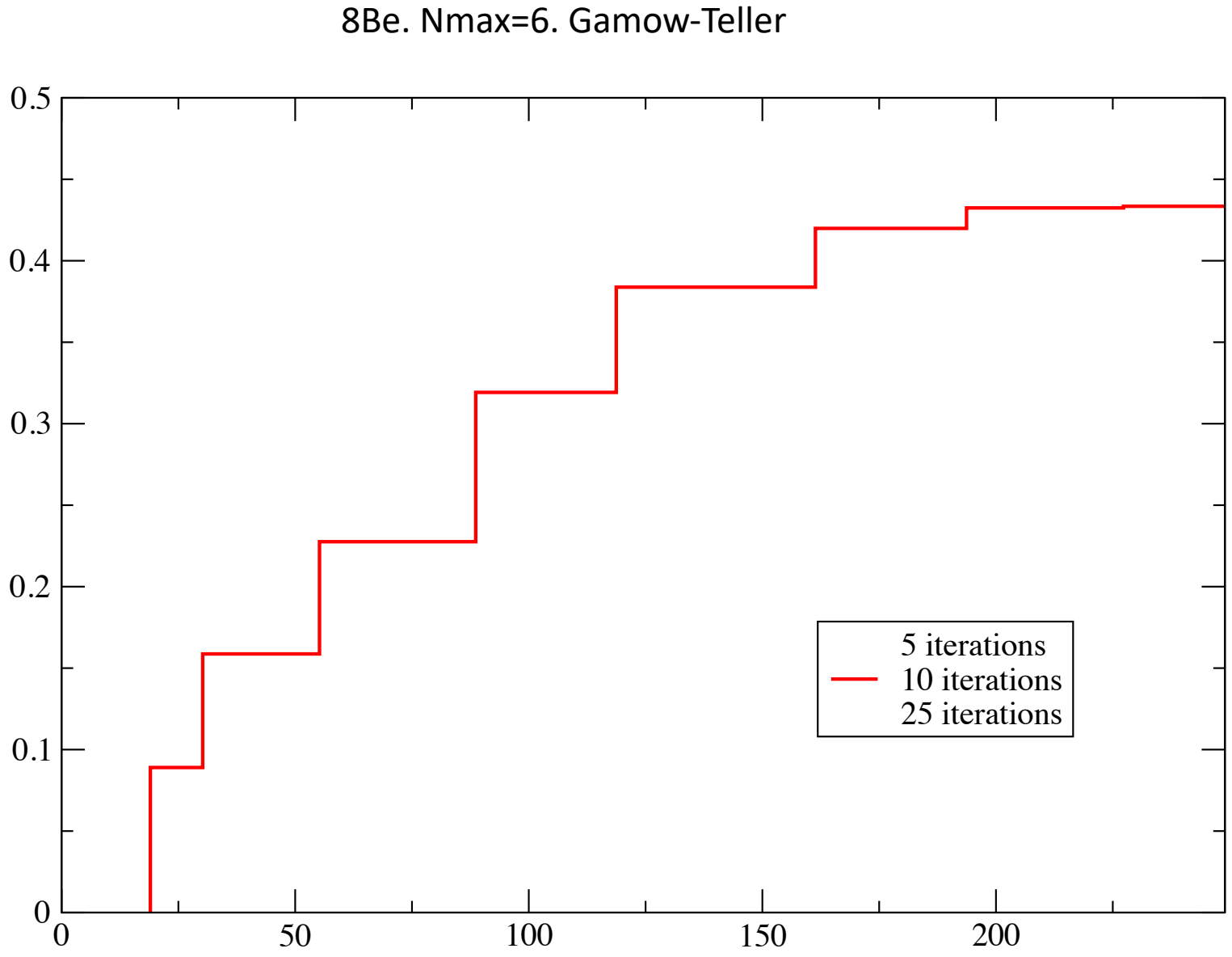
Possible solutions:

- Fold with Gaussian (result depends upon width)
- Lorentz integral transform (best with large number, i.e., many 100's, of iterations)
- **Use running sum**


8Be. Nmax=6. Gamow-Teller
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
5 iterations
10 iterations
25 iterations


8Be. Nmax=6. Gamow-Teller
0.5
0.4
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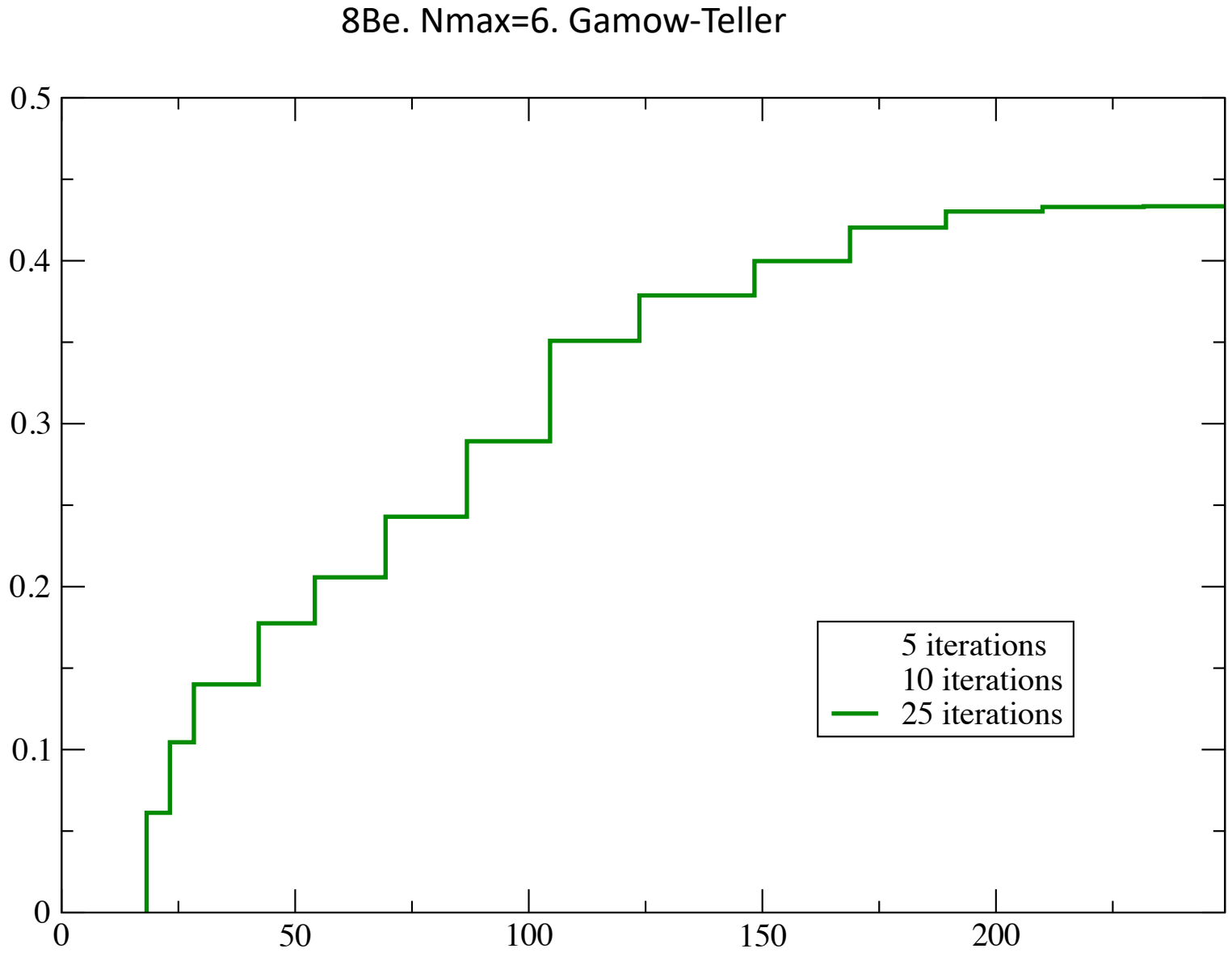
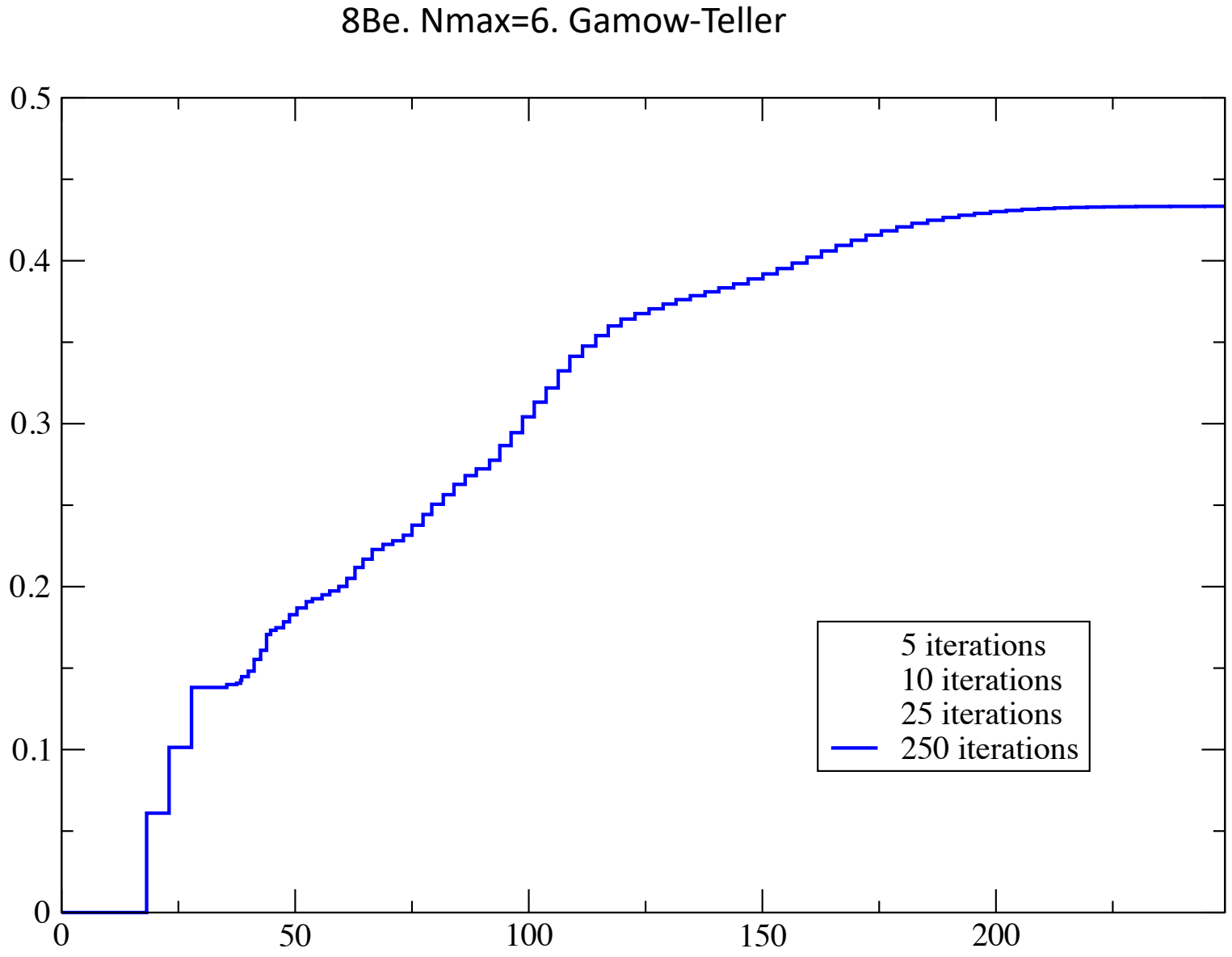
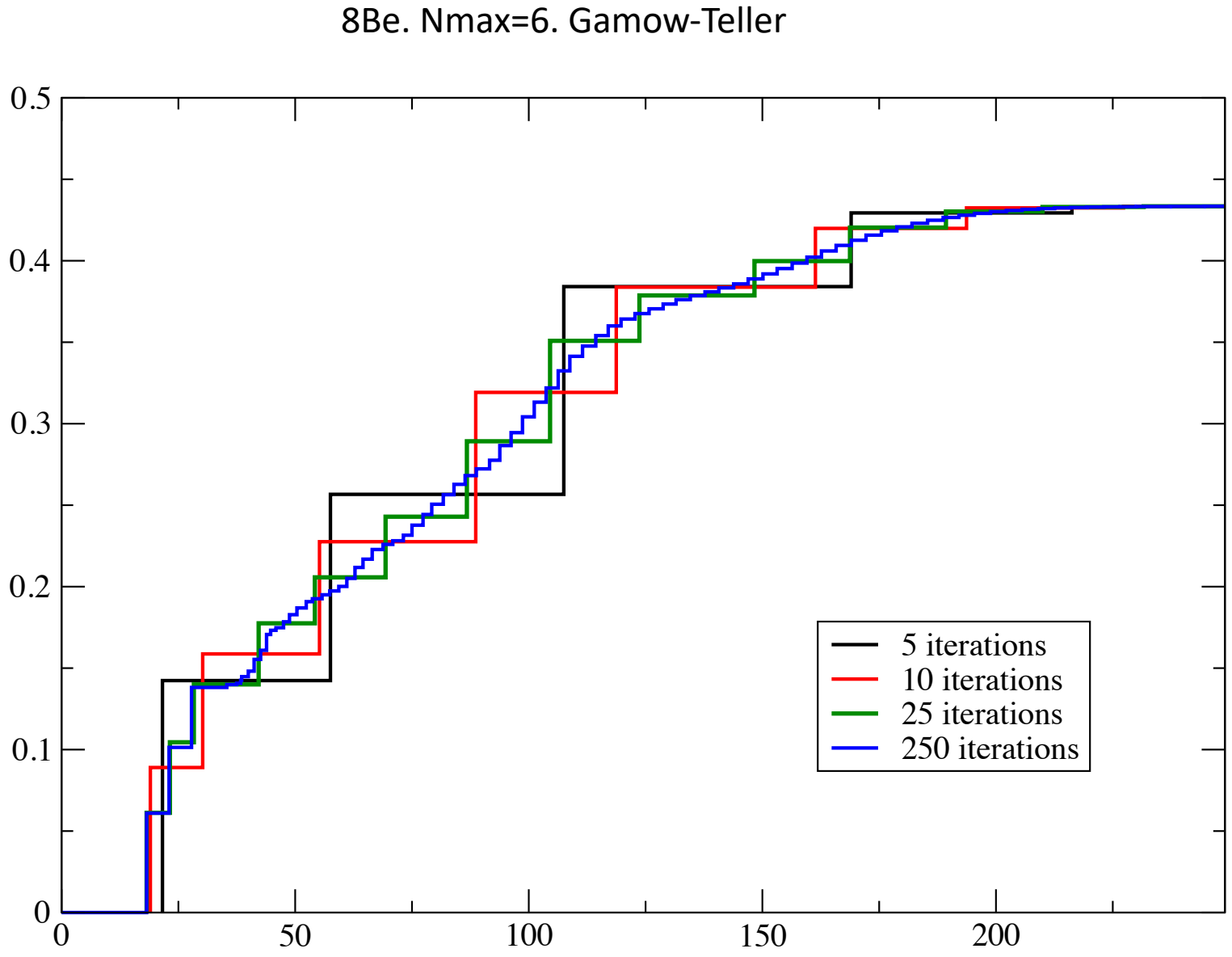
0.2
0.1
0
0
50
100
150
200
5 iterations
10 iterations
25 iterations


8Be. Nmax=6. Gamow-Teller
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
5 iterations
10 iterations
25 iterations


8Be. Nmax=6. Gamow-Teller
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
5 iterations
10 iterations
25 iterations
250 iterations


8Be. Nmax=6. Gamow-Teller
0.5
0.4
0.3
0.2
0.1
0
0
50
100
150
200
5 iterations
10 iterations
25 iterations
250 iterations

The Lanczos trick for strength functions

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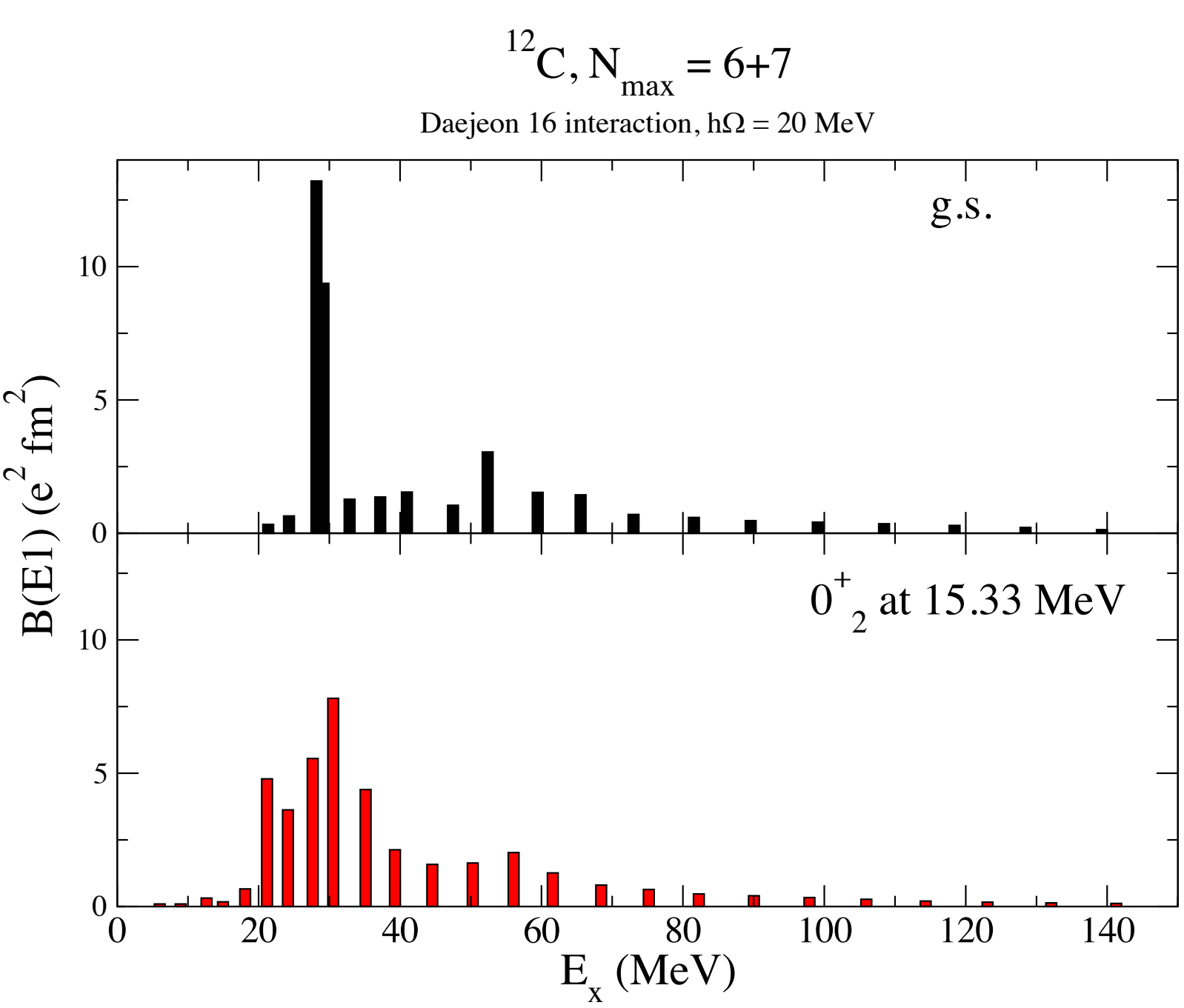
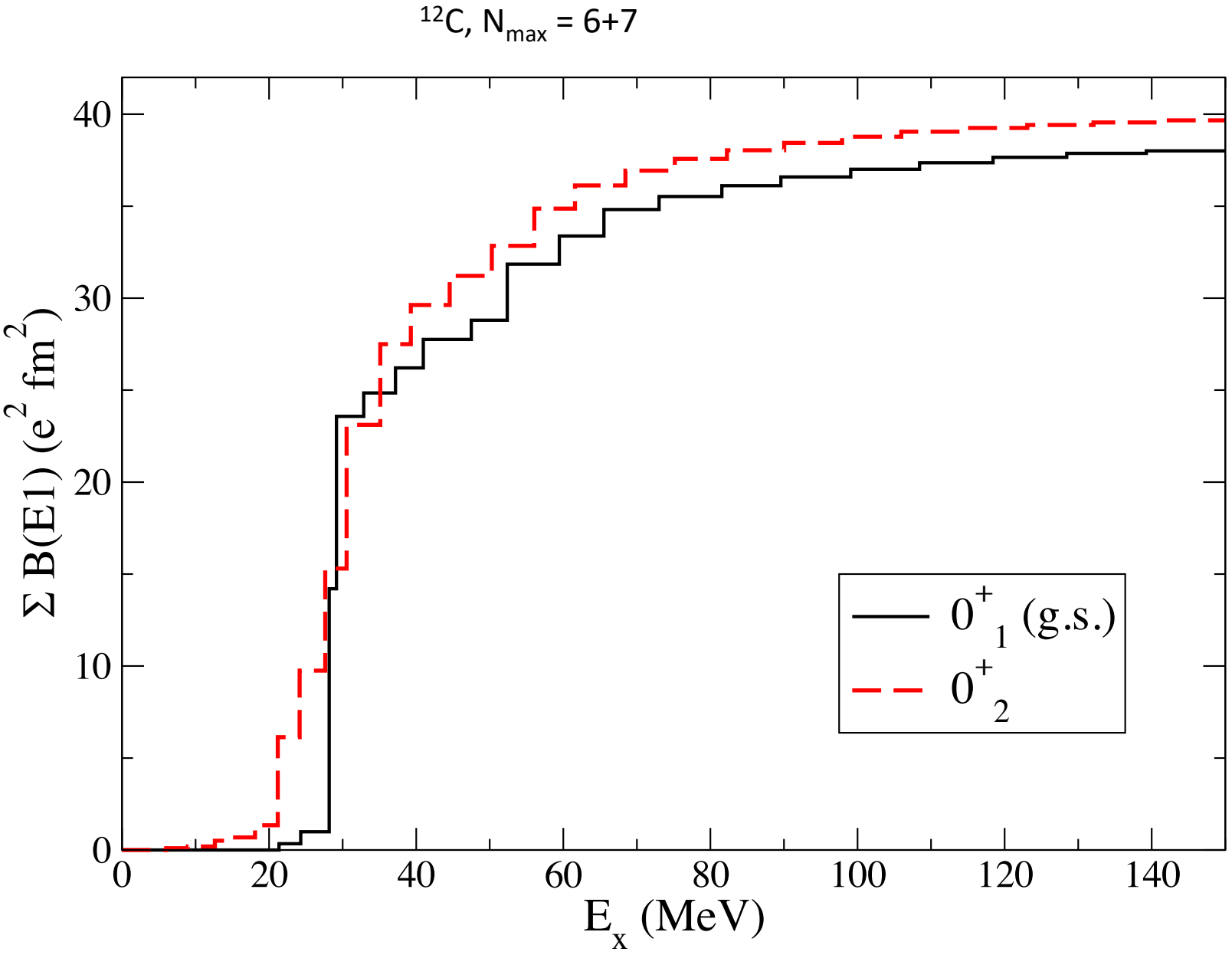
Possible solutions:

- Fold with Gaussian (result depends upon width)
- Lorentz integral transform (best with large number, i.e., many 100's, of iterations)
- **Use running sum**

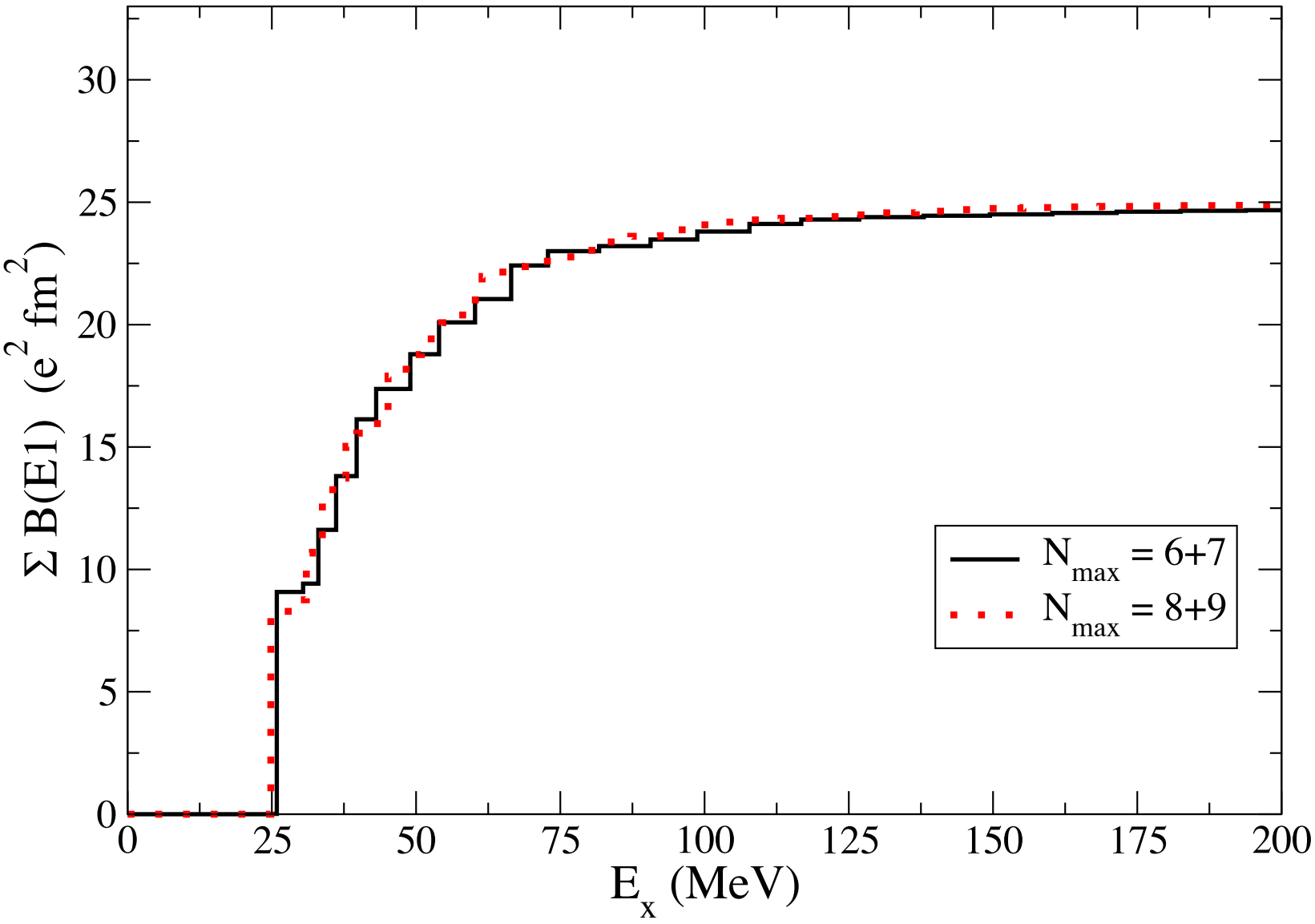
This works because Lanczos generates exact moments of the strength function (2n-1 for n iterations)

See e.g. Whitehead in *Theory and Applications of Moment Methods in Many-Fermion Systems*, 235 (1980)

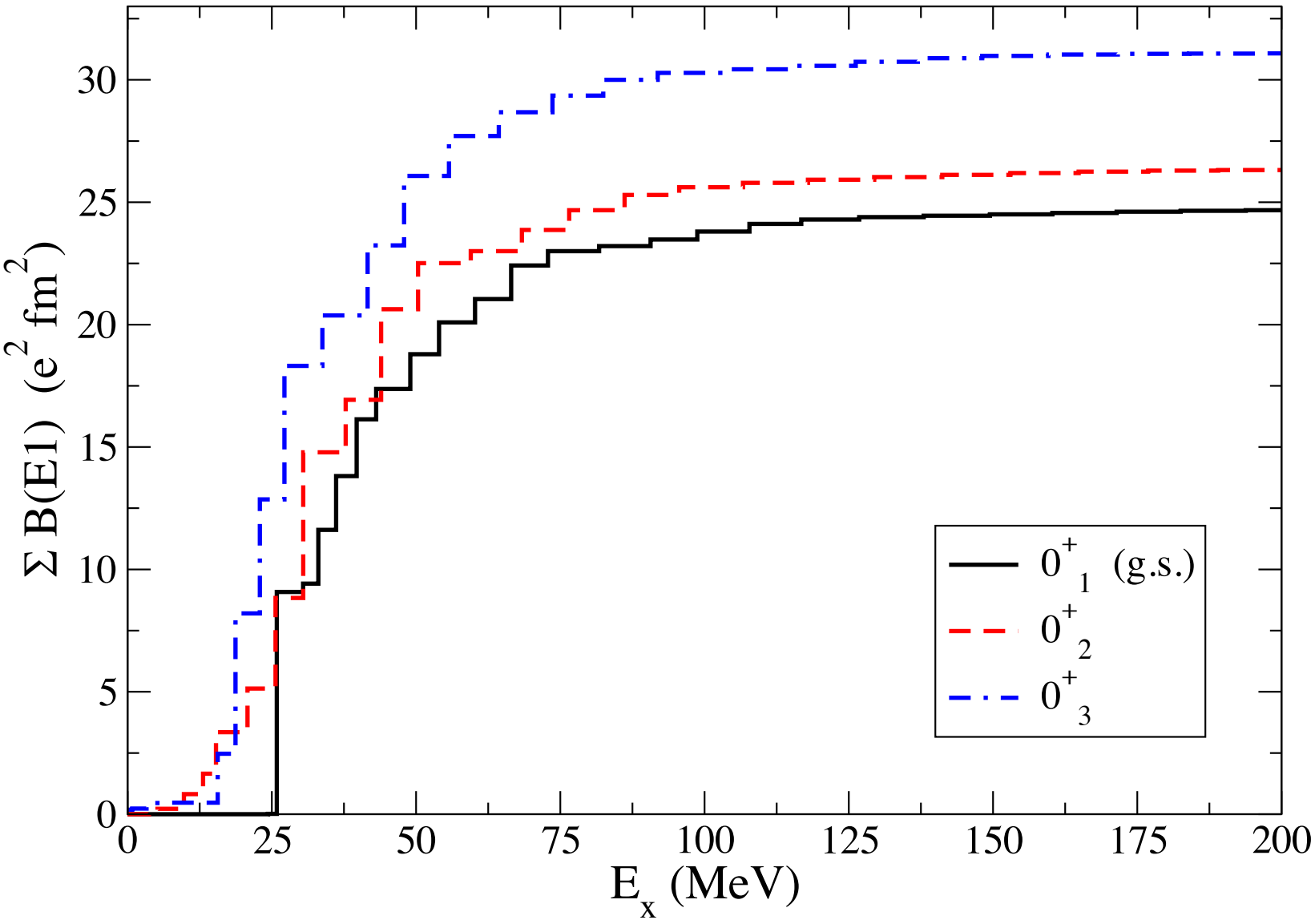

^{12}C, N$_{max}$ = 6+7
Daejeon 16 interaction, hΩ = 20 MeV
g.s.
0^+_2 at 15.33 MeV
B(E1) (e^2 fm^2)
E$_x$ (MeV)
0
5
10
0
20
40
60
80
100
120
140


^{12}C, N_{max} = 6+7
Σ B(E1) (e^2 fm^2)
E_x (MeV)
0
10
20
30
40
0
20
40
60
80
100
120
140
0^+_1 (g.s.)
0^+_2

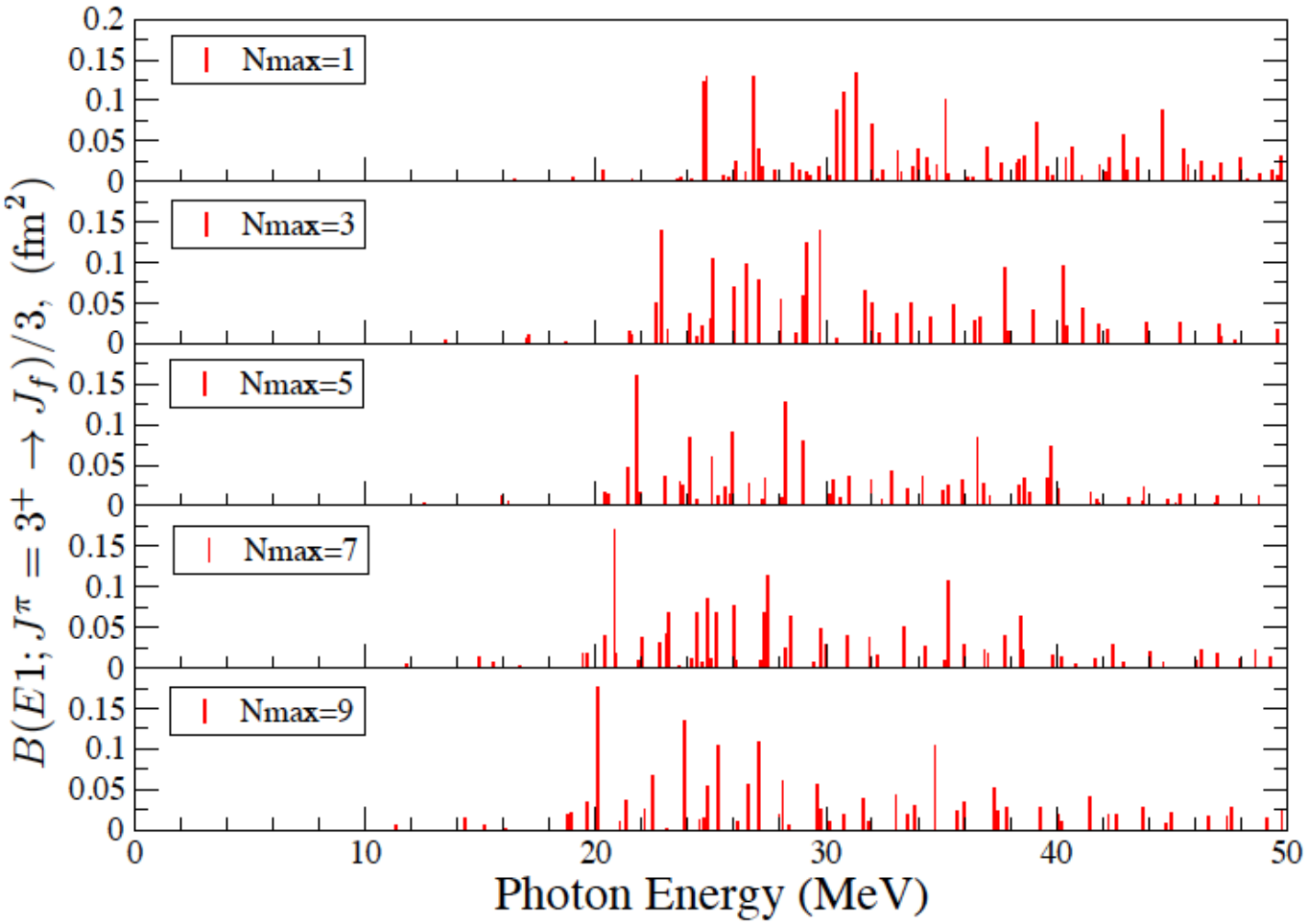
^{8}Be g.s. strength function



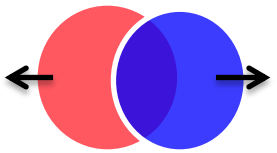
^{8}Be g.s. strength function



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

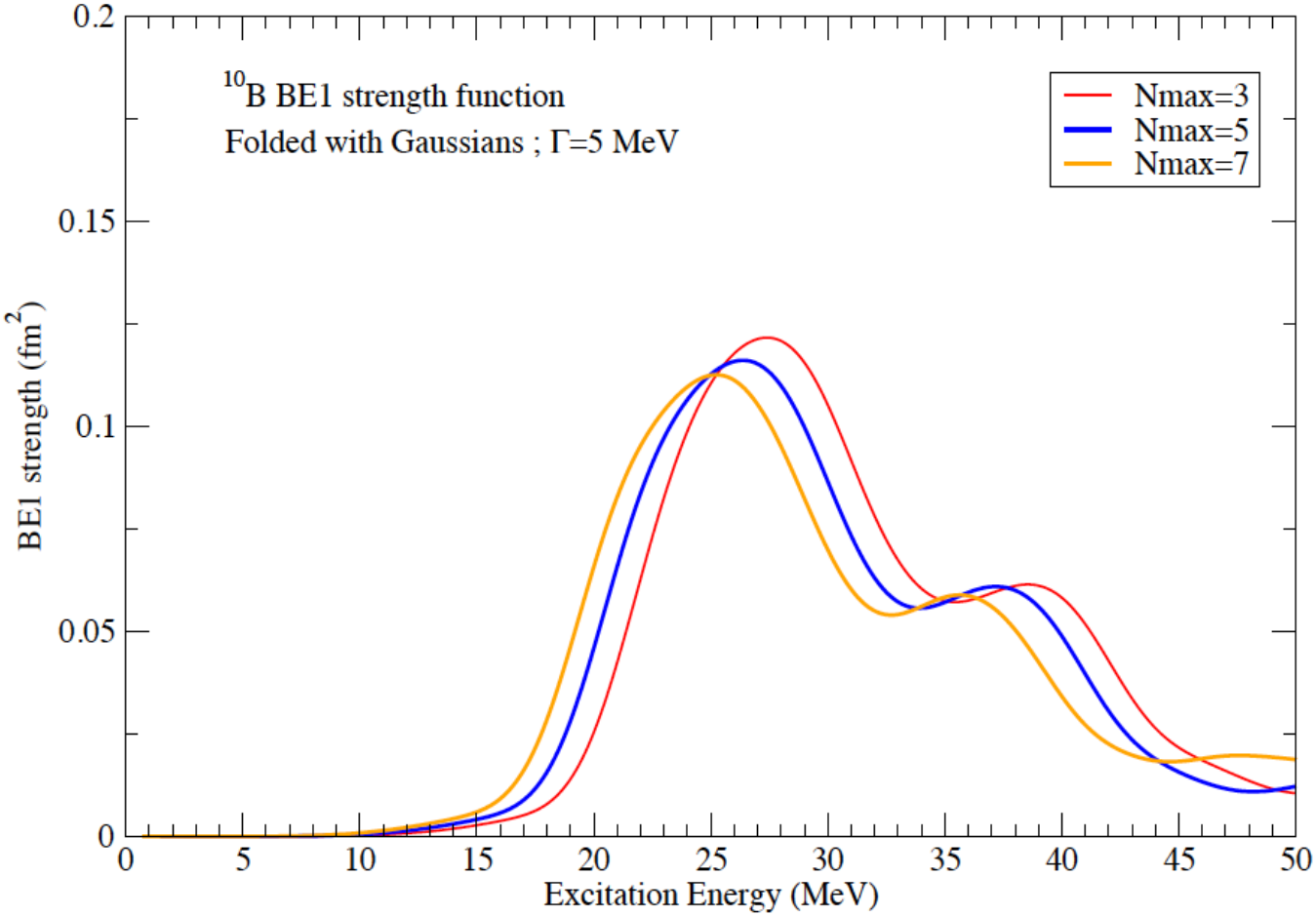


^{10}B E1 response



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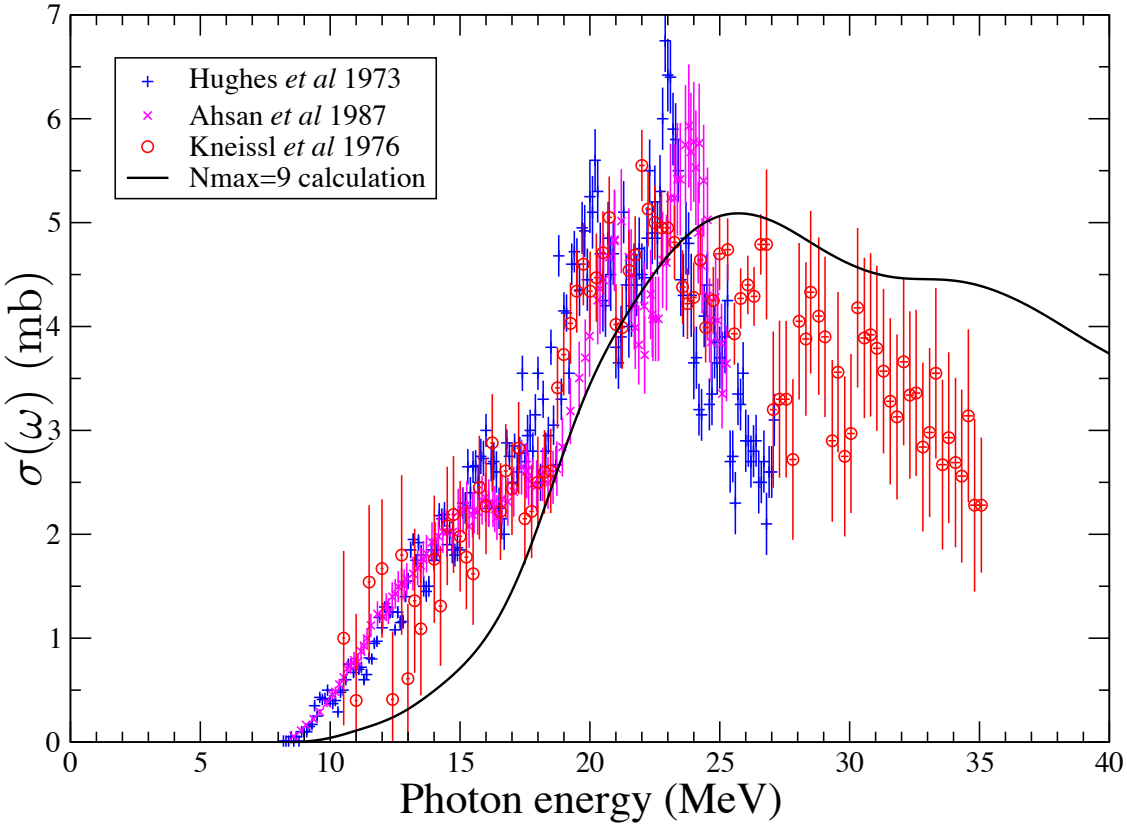
Kruse, Ormand, and Johnson: arXiv:1502:03464



^{10}B E1 response

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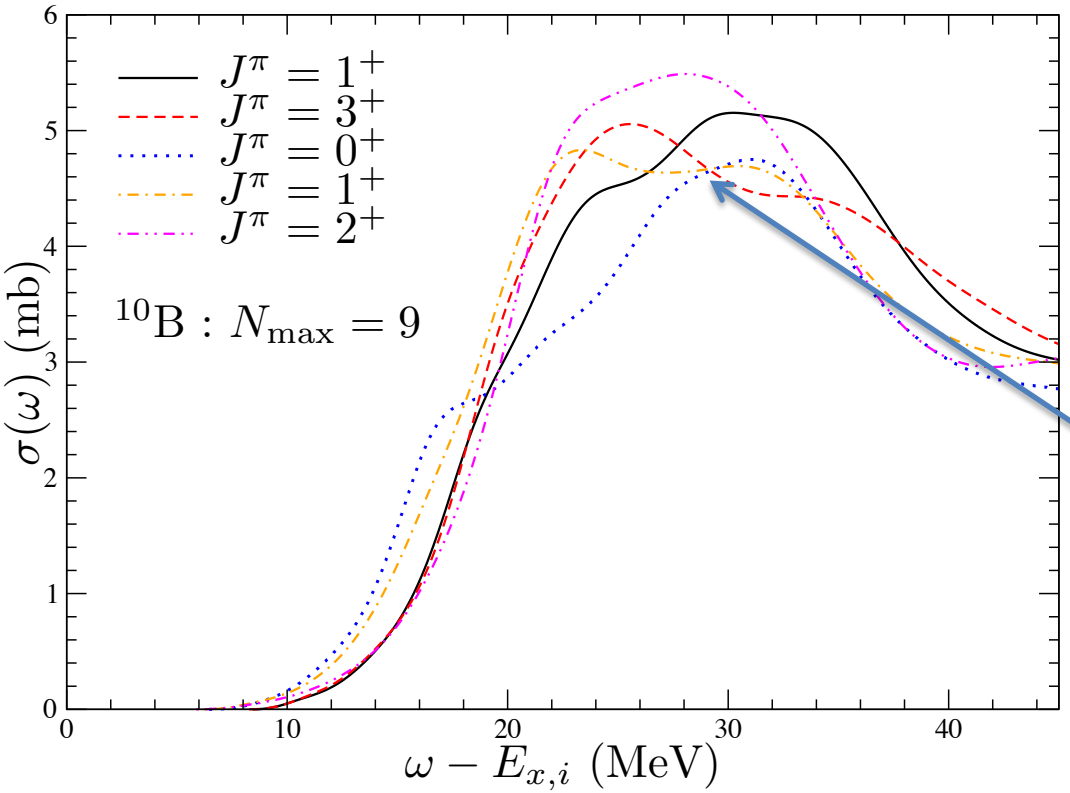
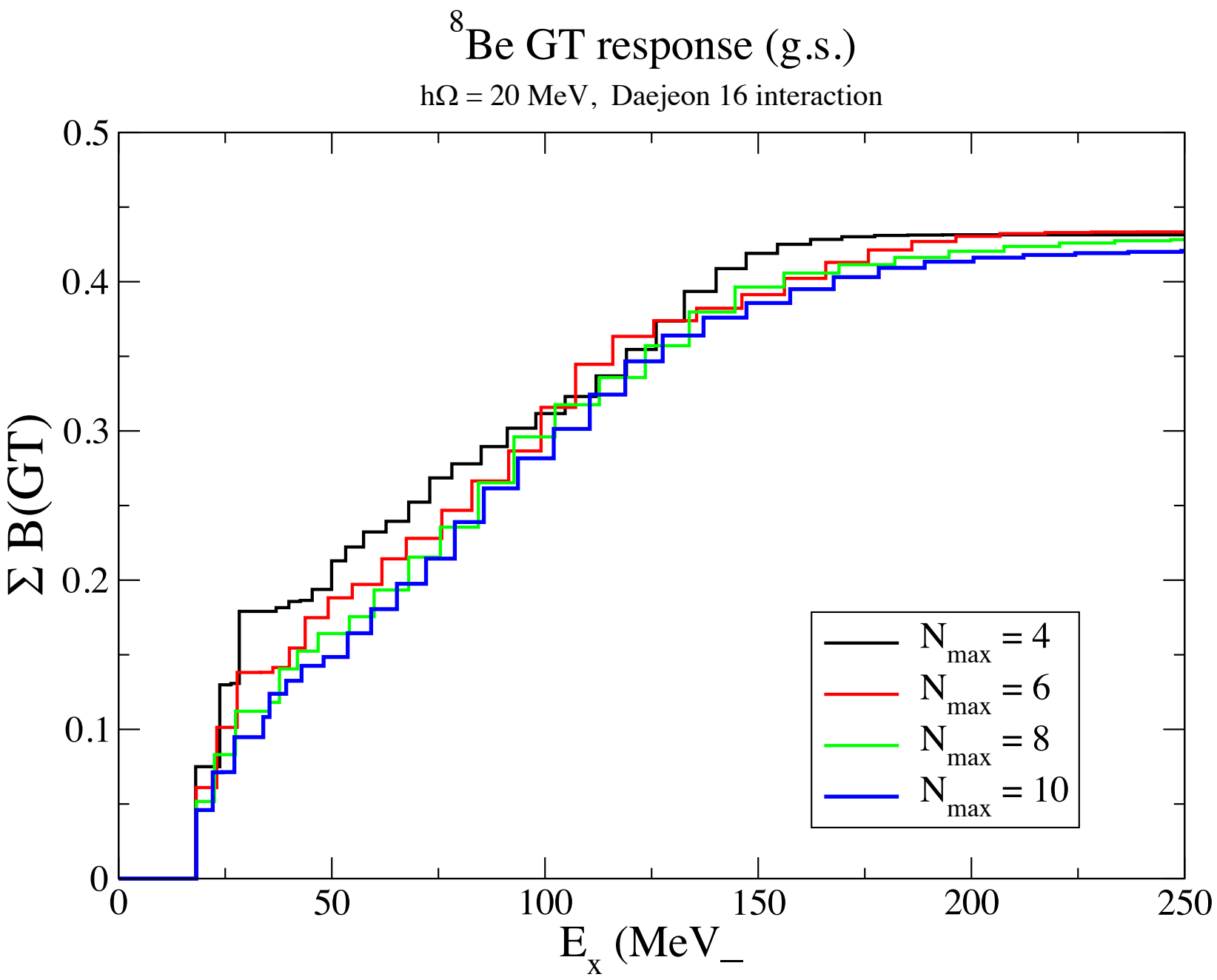


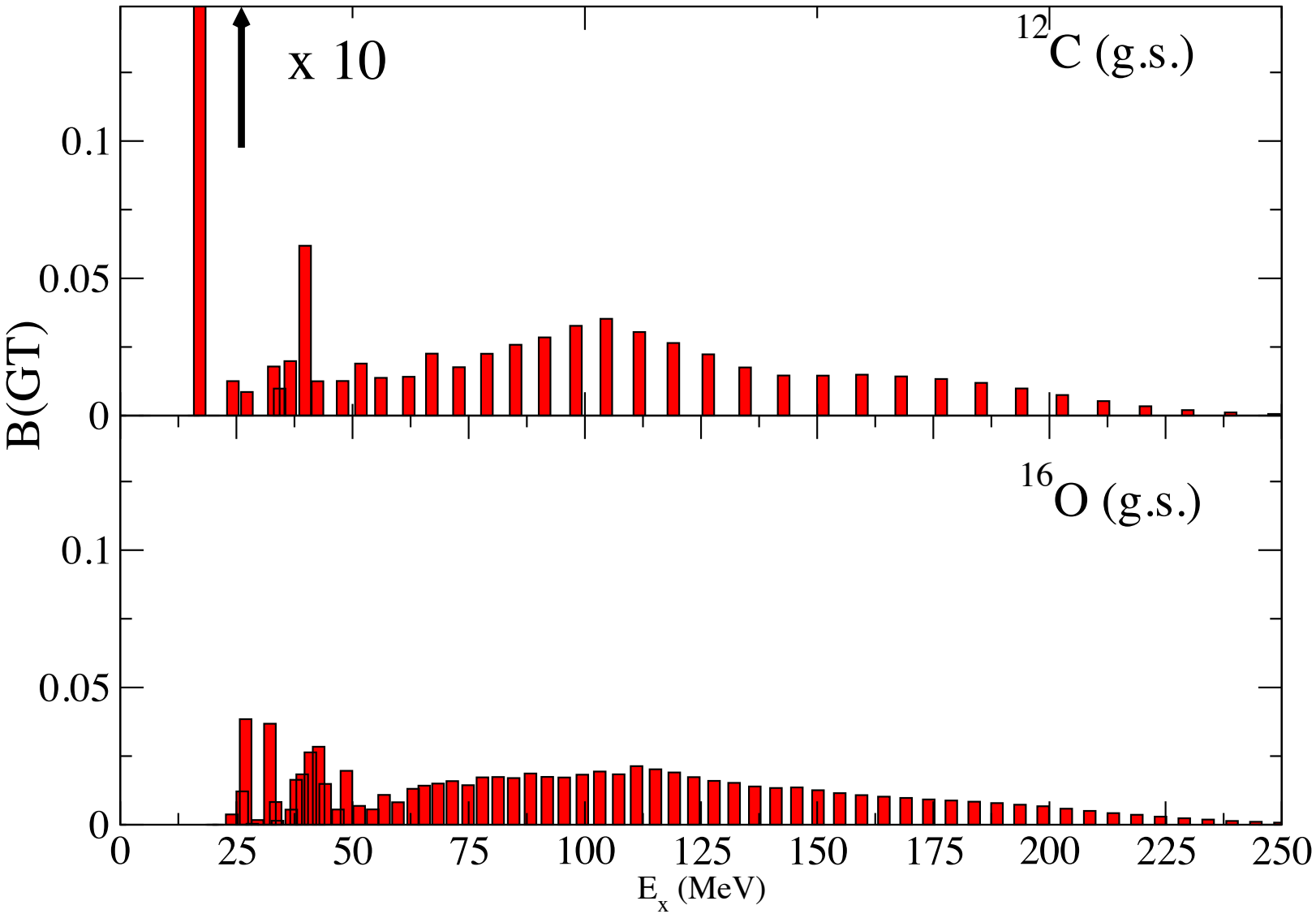
^{10}B E1 response

GDR

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


^{8}Be GT response (g.s.)
hΩ = 20 MeV, Daejeon 16 interaction
Σ B(GT)
E$_x$ (MeV_
0
0.1
0.2
0.3
0.4
0.5
0
50
100
150
200
250
N$_{max}$ = 4
N$_{max}$ = 6
N$_{max}$ = 8
N$_{max}$ = 10

N_{max} = 6 calculations



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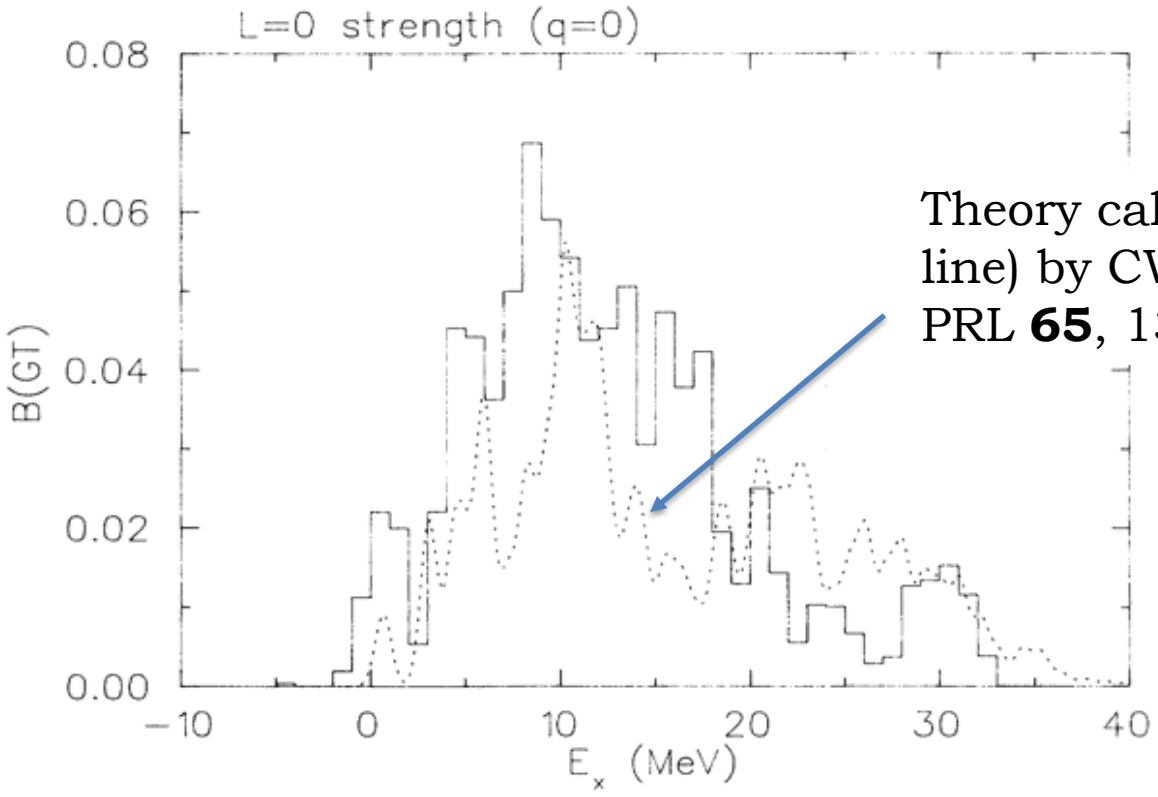
^{16}O B(GT) experimentally measured via *(n,p)* at TRIUMF!
Hicks *et al* PRC **43**, 2554 (1991)



Theory calculation (dotted line) by CWJ & Haxton, PRL **65**, 1325 (1990)

Strength function sum rules

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A shorthand for strength functions are sum rules,

e.g., the *non-energy-weighted sum rule*, or total strength,

$$S_0 = \int S(E)dE = \sum_f \left|\langle f|\hat{O}|i\rangle\right|^2$$

and the *energy-weighted sum rule*

$$S_1 = \int S(E)E\,dE = \sum_f (Ef - Ei)\left|\langle f|\hat{O}|i\rangle\right|^2$$

Strength function sum rules

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A shorthand for strength functions are sum rules,

One can evaluate the NEWSR and EWSR as expectation values of operators:

$$S_0 = \langle i | \hat{O}^\dagger \hat{O} | i \rangle$$

$$S_1 = \frac{1}{2} \left\langle i \middle| \left[\hat{O}^\dagger, [\hat{H}, \hat{O}] \right] \middle| i \right\rangle$$

A special case is the Thomas-Reiche-Kuhn sum rule, which is the EWSR for E1.

Strength function sum rules

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A shorthand for strength functions are sum rules,

One can evaluate the NEWSR and EWSR as expectation values of operators:

$$S_0 = \langle i | \hat{O}^\dagger \hat{O} | i \rangle$$

$$S_1 = \frac{1}{2} \left\langle i \middle| \left[\hat{O}^\dagger, [\hat{H}, \hat{O}] \right] \middle| i \right\rangle$$

Such operators may be useful when it is difficult to carry out full Lanczos (IT-NCSM? CC?)

Strength function sum rules

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A shorthand for strength functions are sum rules,

One can evaluate the NEWSR and EWSR as expectation values of operators:

$$S_0 = \langle i | \hat{O}^\dagger \hat{O} | i \rangle$$

$$S_1 = \frac{1}{2} \left\langle i \left| \left[\hat{O}^\dagger, [\hat{H}, \hat{O}] \right] \right| i \right\rangle$$

The matrix elements for general operators (both **O** and **H**) and a computer program written:

Yi Lu (Qufu Normal University) and CWJ, arxiv.org:1710.03187

^{16}O B(GT) experimentally measured via *(n,p)* at TRIUMF!
Hicks *et al* PRC **43**, 2554 (1991)

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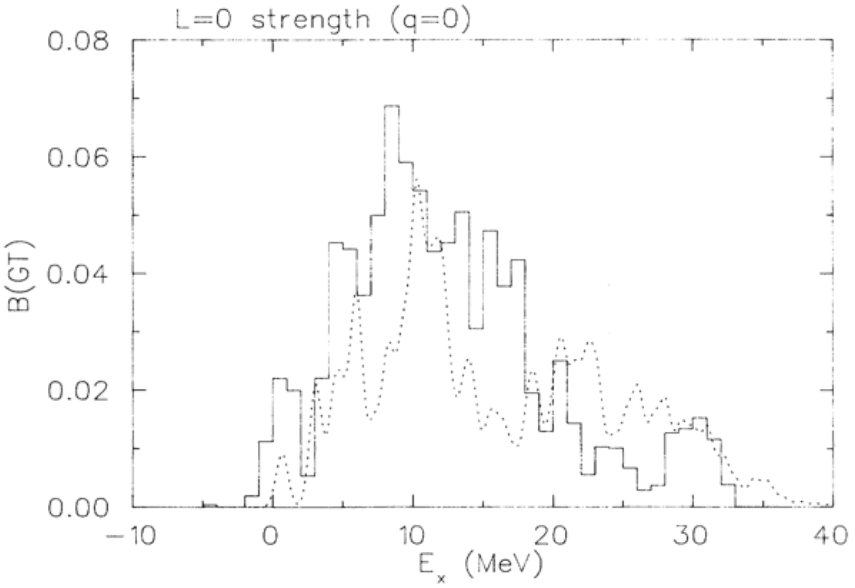

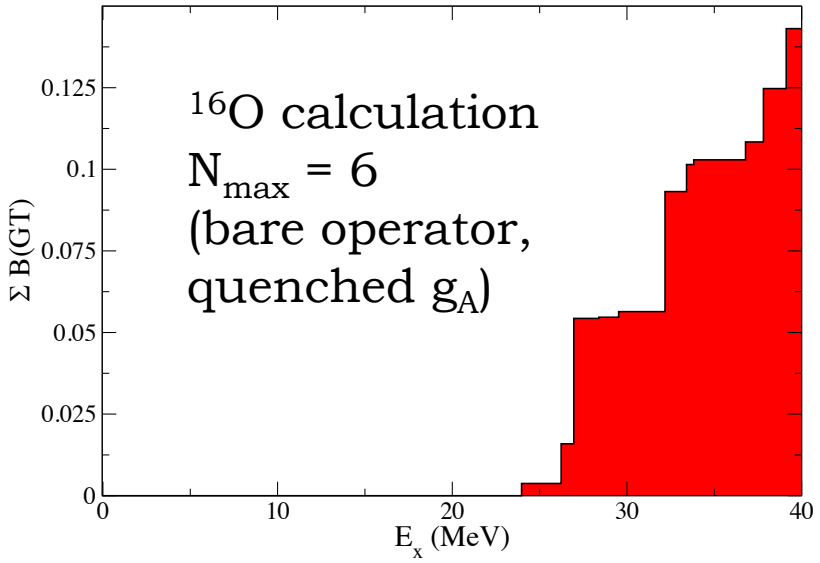

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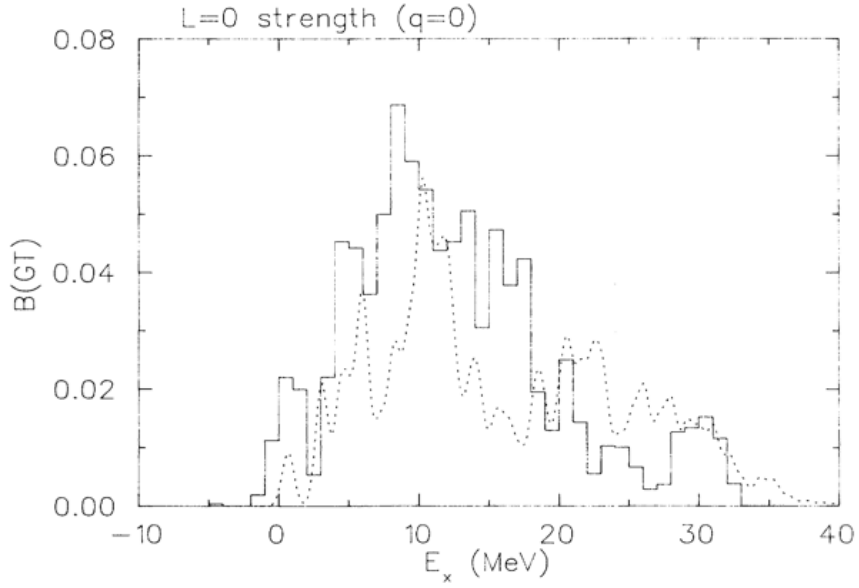
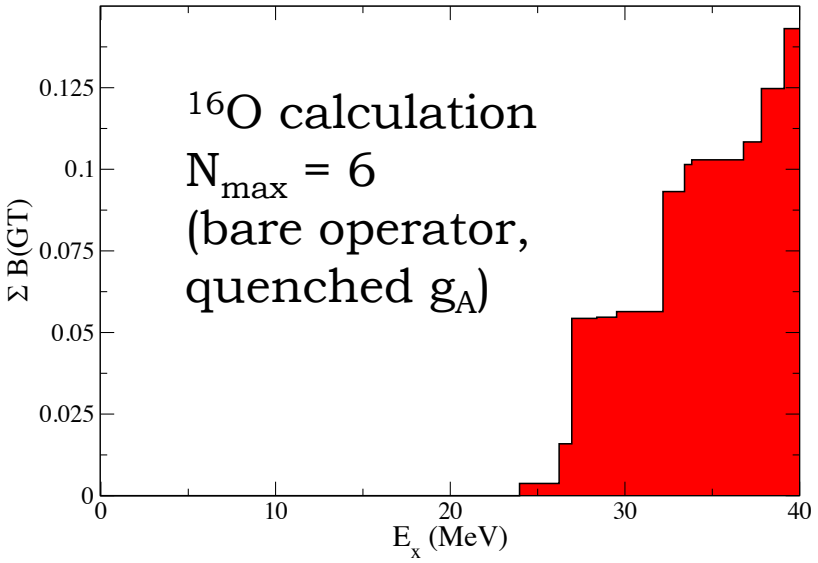
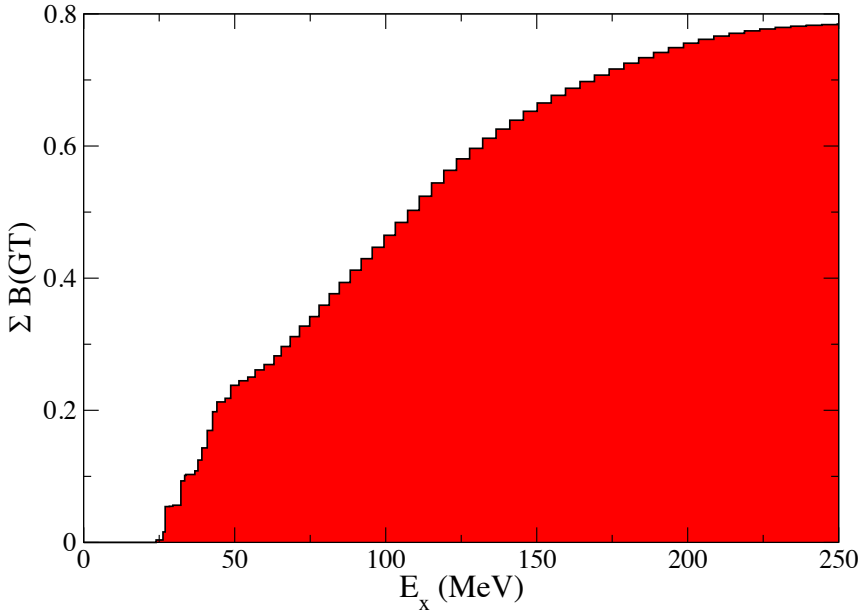


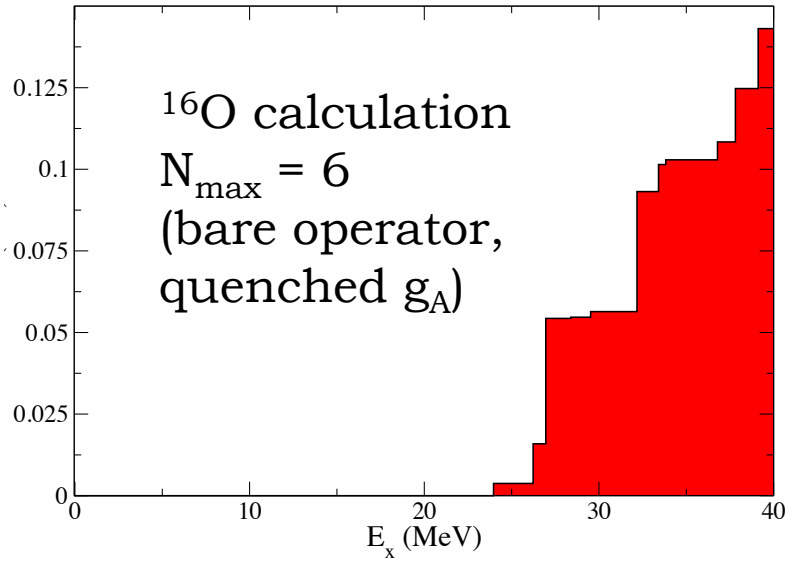


Experimental result: sum B(GT) up to 40 MeV ~ 0.7-0.8
(Old calculation: 0.66)

NCSM: ~ 0.14 up to 40 MeV, ~ 0.8 up to 250 MeV

^{16}O B(GT) experimentally measured via *(n,p)* at TRIUMF!
Hicks *et al* PRC **43**, 2554 (1991)





Experimental result: sum B(GT) up to 40 MeV ~ 0.7-0.8
(Old calculation: 0.66)

NCSM: ~ 0.14 up to 40 MeV, ~ 0.8 up to 250 MeV

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The total B(GT) strength measures the smearing of the Fermi surface about the closed core.

Failure of the NCSM calculation for ^{16}O is probably related to lack of clustering a la Hoyle state in ^{12}C

It would be **very interesting** for other methods, e.g., coupled-cluster, IT-NCSM for large N_{max}, to compute these sum rules for Gamow-Teller in ^{16}O!

Ongoing work

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More application of strength functions and strength function sum rules in NCSM.

In particular looking at

- Tests of Brink-Axel hypothesis (can compute sum rules for many levels quickly)
- Comparison of E1 EWSR against TRK sum rule ('momentum-dependent' part of interaction)