HPNC in ^{18}F:
Modern shell-model *opportunities*

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N3AS workshop on HPNC @ KITP, March 2018

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Hadronic parity nonconservation is *tiny*.
Need either *very* sensitive measurements…
..or a good amplification!

PNC amplitude = $\frac{\langle \psi_- | \hat{H}_{PNC} | \psi_+ \rangle}{E_- - E_+}$

(in 1st order perturbation theory)

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So… look for nearby parity doublets!

The HPNC “gang of four”:

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^{14}N

^{18}F

^{19}F

^{21}Ne

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The HPNC "gang of four":

^{14}N

^{18}F g.s. is 1^+; low-lying 0^+,0^- separated by only 39 keV!

^{19}F

^{21}Ne

Barnes *et al* PRL **40**, 840, 1980

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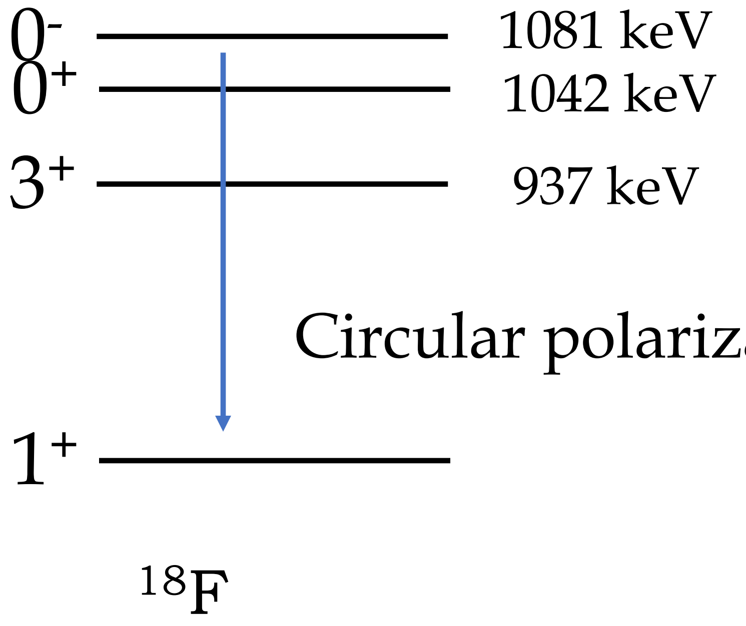

Circular polarization ~ (-0.7$\pm$2.0)$\times 10^{-3}$

Adelberger *et al* PRL **46**, 695, 1981

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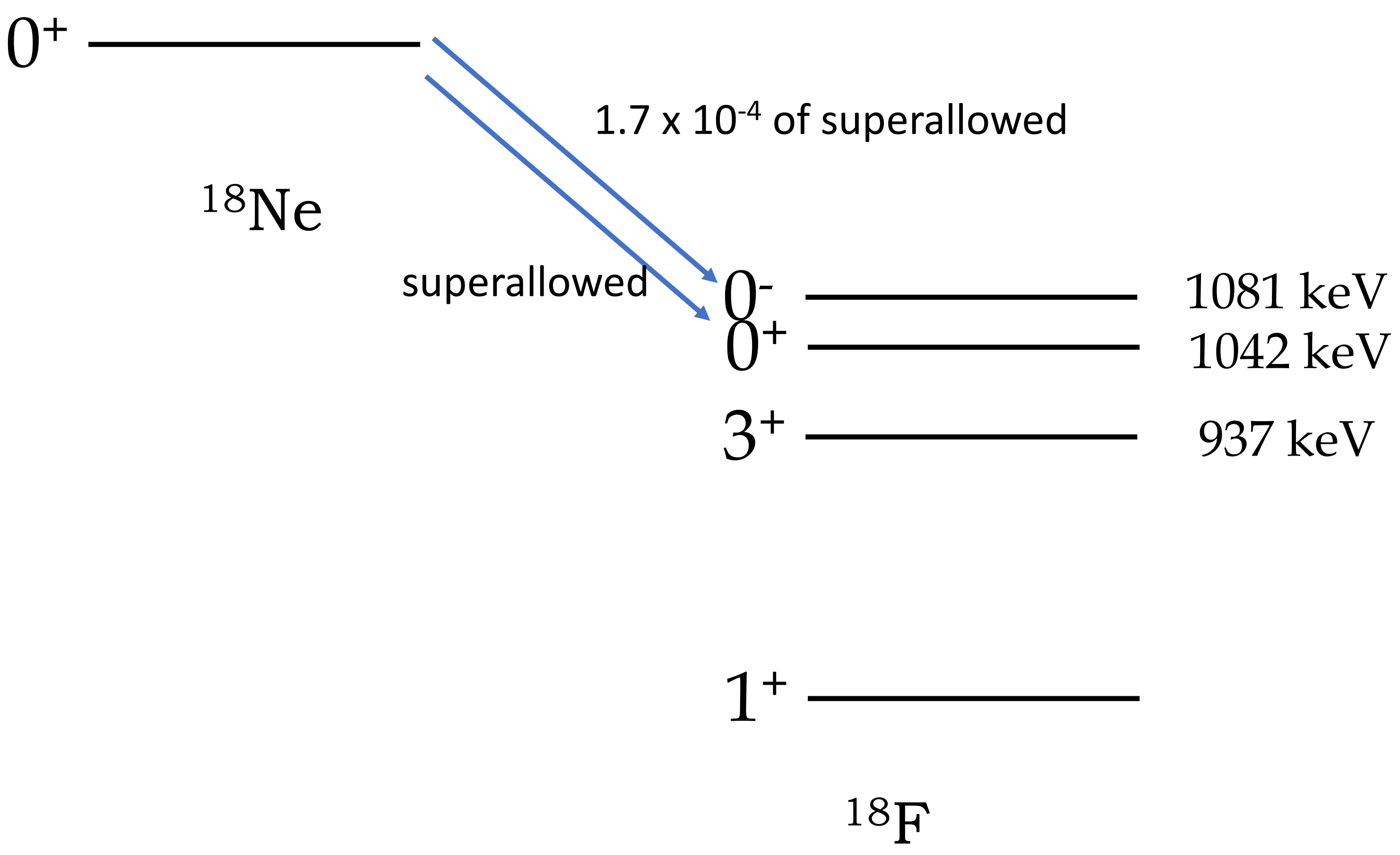

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^{18}F

g.s. is 1^+; low-lying 0^+,0^- separated by only 39 keV! -> mixing in γ decay

2-body current tricky to compute, although with new *ab initio* methods (χ EFT or lattice QCD) now better.

Old idea: relate 2-body 0^- operator to 1-body ops $\vec{\sigma} \cdot \vec{r}$, $\vec{\sigma} \cdot \vec{\nabla}$ (1st forbidden axial vector (Gamow-Teller))

See Haxton PRL **46**, 698 (1981), Haxton +CWJ, PRL **65**, 1325 (1990)

Configuration-interaction shell model

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Flexible microscopic model with *ab initio* foundations

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"Diagonalize once and get lots of eigenvalues" --KN

Configuration-interaction shell model

Flexible microscopic model with *ab initio* foundations

Basic idea: (1) compute matrix elements of modern two-body PNC operators and check robustness (e.g., with model space, interaction), and
(2) check proportionality hypothesis between 2- and 1-body operators

THE BASIC PROBLEM

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The basic *science question* is to model detailed quantum structure of many-body systems, such the structure of an atomic nucleus.

To answer this, we solve *Schrödinger's equation*:

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

* **H** is generally a very large matrix – dimensions up to 10^{10} have been tackled.
* **H** is generally very sparse.
* We usually only want a few low-lying states

The Basic Problem

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

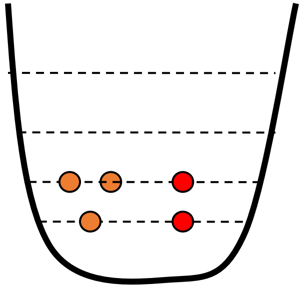
$$\sum_\beta H_{\alpha\beta} c_\beta = E c_\alpha \quad \text{if} \quad \langle\alpha|\beta\rangle = \delta_{\alpha\beta}$$

so we use the matrix formalism

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

Nuclear Hamiltonian: $\hat{H} = \sum_i -\frac{\hbar^2}{2M}\nabla_i^2 + \sum_{i<j} V(r_i, r_j)$

Solve by diagonalizing **H** in a basis of many-body states.
The many-body states are *Slater determinants*, or anti-symmeterized products of single-particle wfns.



The single-particle states are defined by a single-particle potential *U(r)* (such as harmonic oscillator or Hartree-Fock)

Maria Mayer

At this point one generally goes to occupation representation:

$$\hat{H} = \sum_i \varepsilon_i \hat{a}_i^+ \hat{a}_i + \frac{1}{4}\sum_{ijkl} V_{ijkl} \hat{a}_i^+ \hat{a}_j^+ \hat{a}_l \hat{a}_k$$

single-particle energies

two-body matrix elements

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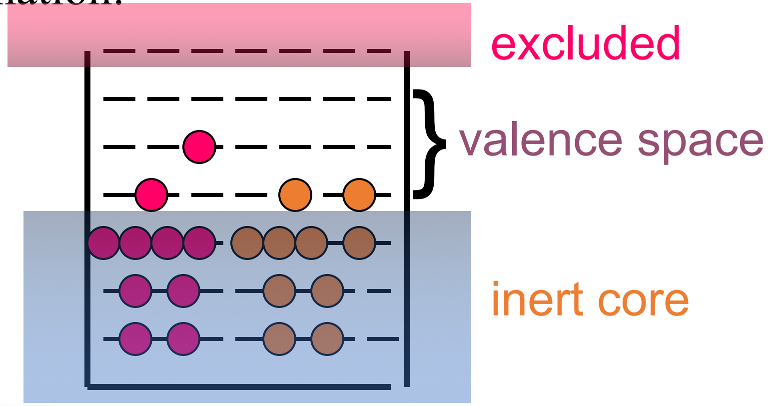
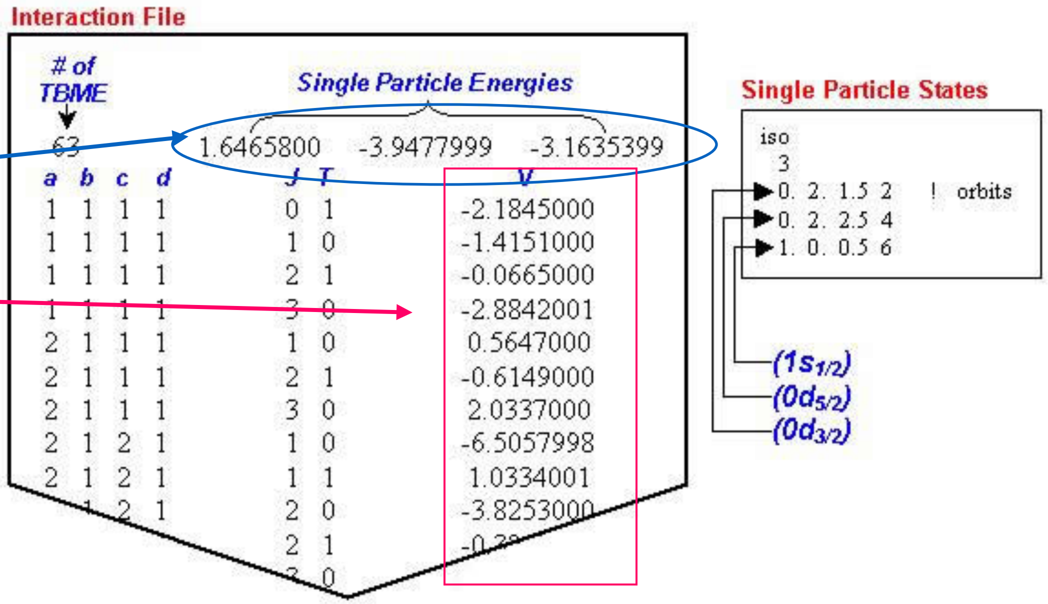
When running a fermion shell model code (e.g. MFD, BIGSTICK), one enters the following information:

(1) The single-particle valence space (such as *sd* or *pf*); assumes inert core



(2) The many-body model space (number of protons and neutrons, truncations, etc.)

(3) The interaction:
single-particle energies
and
two-body matrix elements
$V_{JT}(ab,cd)$



Not your grandfather's shell model

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Old shell model: good description of data, but (detailed) phenomenological

Today's shell model: rigorous starting from high precision nuclear forces
Good agreement *without fitting* to many data points

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Today's shell model: rigorous starting from high precision nuclear forces
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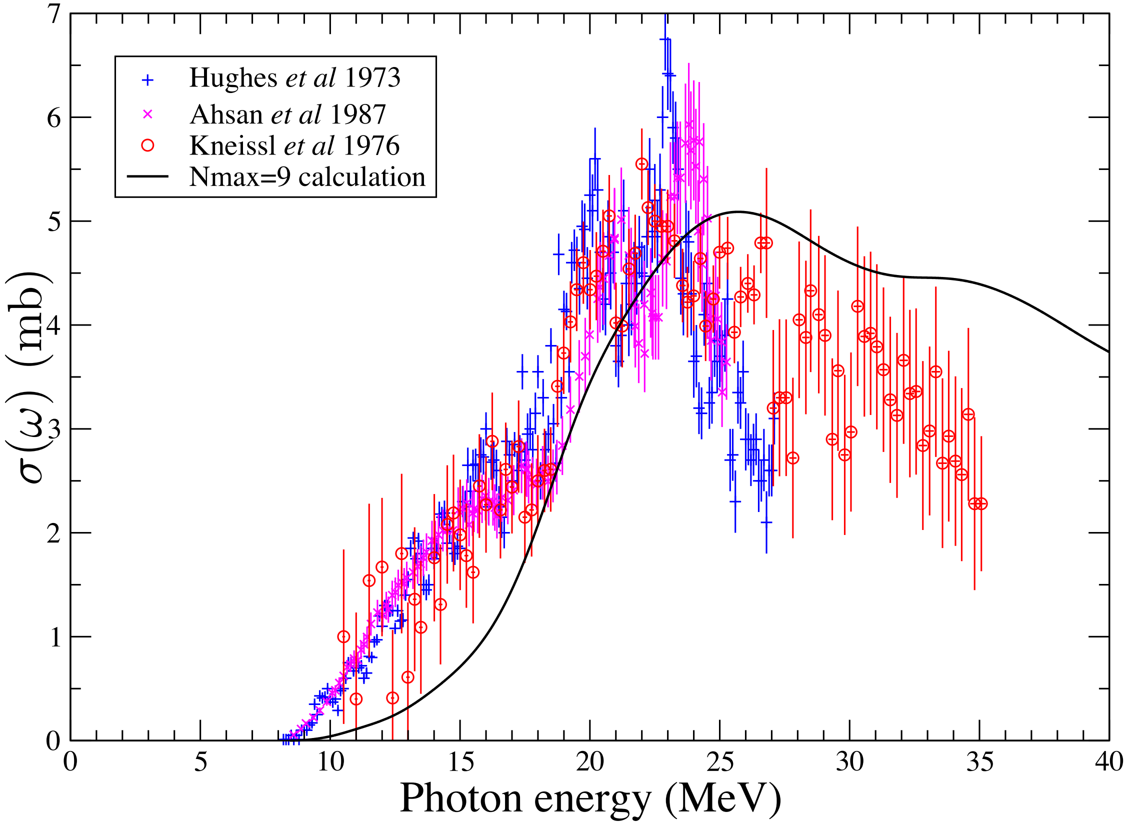
(energy levels of light nuclei, scattering in light systems, ^{14}C half-life!)

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



^{10}B E1 response

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Not your grandfather's shell model

NN data -> high precision description of nuclear forces
e.g. Argonne potential, chiral EFT, phase-equivalent potentials (JISP, Daejeon)

Note: these all agree on phase shifts, deuteron binding = on shell matrix elements
Differ on off-shell matrix elements -> three-body forces

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NN data -> high precision description of nuclear forces

Unitary transformations ("similarity renormalization group")
"soften" the hard core = reduce coupling between low and high momentum

These induce additional three (and four) body forces.
Note: main effect is to shift energies down [CWJ, PLB **774**, 465 (2017)]

Not your grandfather's shell model

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NN data -> high precision description of nuclear forces

Unitary transformations "soften" the hard core

No-core shell model space (all particles active) reduces intruder states (some cluster states still intruders, e.g. Hoyle state in ^{12}C, 0^+_2 state in ^{16}O)

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NN data -> high precision description of nuclear forces

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Modern high performance computing allows us to go to much larger spaces.

1989: 4p-4h calculation of ^{16}O dim ~ 1.2 million bases, "state of the art"

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Today: can do N_{max} = 8 for ^{16}O, dim ~ 1 billion bases is "state of the art"
N_{max} = 10, dim = 24 billion bases within sight

The BIGSTICK shell-model code, free and open-source

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Download from:
github.com/cwjsdsu/BigstickPublick

Manual at arXiv:1801.08432

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

The BIGSTICK shell-model code, free and open-source

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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.

^{18}F shell model calculations

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N_{max} = 6 (+ parity) dim 426 million

N_{max} = 7 (- parity) dim 2.7 billion

^{18}F shell model calculations

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N_{max} = 6 (+ parity) dim 426 million

N_{max} = 7 (- parity) dim 2.7 billion

Will study convergence with N_{max} = max # of oscillator quanta

Can also try 'natural orbits' (cf. M. Caprio, R. Roth) which improve convergence, robustness in choice of h.o. basis

^{19}F shell model calculations

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N_{max} = 6 (+ parity) dim 1.3 billion

N_{max} = 7 (- parity) dim 8.5 billion

^{21}Ne shell model calculations

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N_{max} = 6 (+ parity) dim 11.5 billion

N_{max} = 7 (- parity) dim 71.5 billion!

more practical

N_{max} = 4 (+ parity) dim 194 million

N_{max} = 5 (- parity) dim 1.6 billion!

$\alpha + p/n$ shell model calculations

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N_{max} = 20 (- parity) dim 600 million

N_{max} = 21 (+ parity) dim 1 billion!

^{18}F shell model calculations

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A big concern I have: correct 4p-4h states in wave functions.

^{18}F shell model calculations

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A big concern I have: correct 4p-4h states in wave functions.

Near the p-sd boundary, we see strong 4p-4h correlations. These include the famous Hoyle state in ^{12}C
and the analogous 0^+_2 state at 6 MeV in ^{16}O.

No-core shell model calculations have these too high in the spectra. These probably cannot be arrived at by brute force.

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

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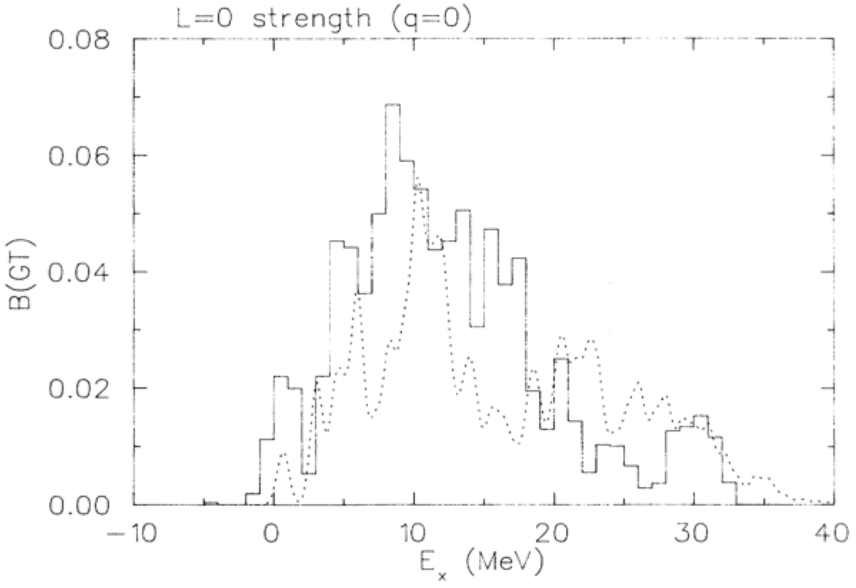

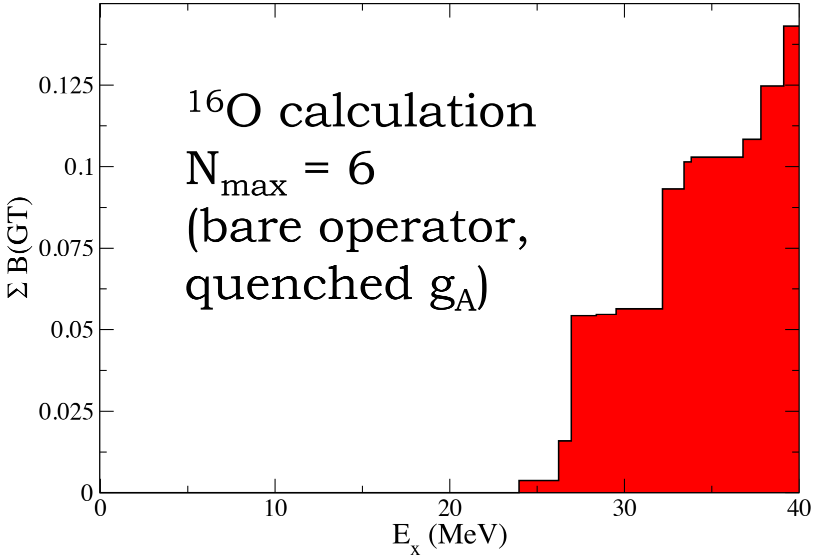

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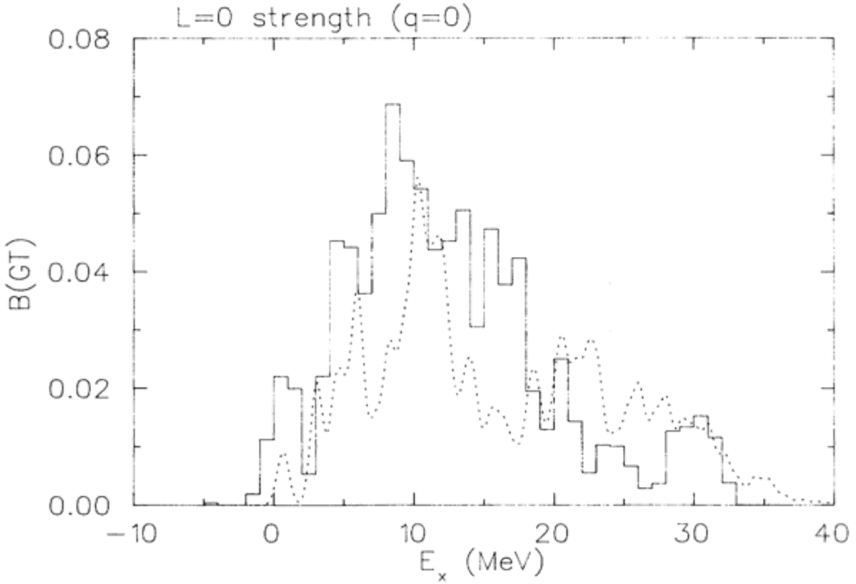

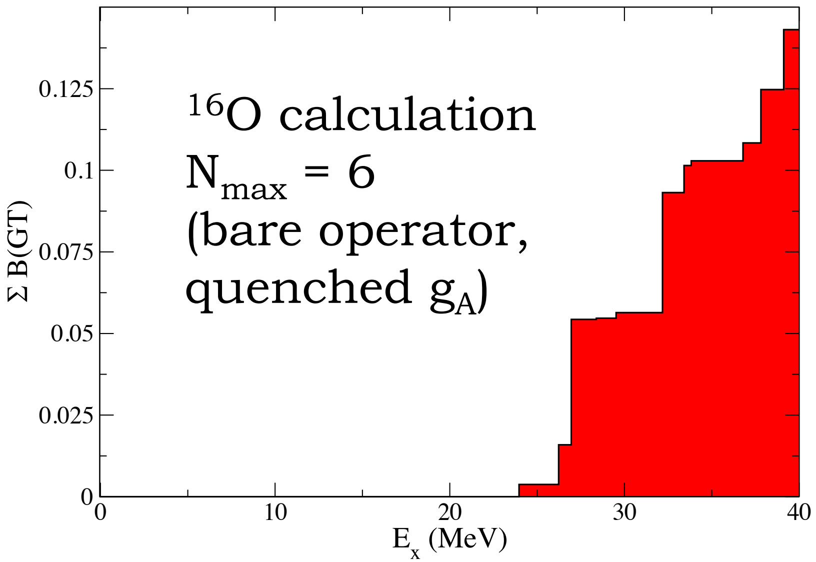

Experimental result: sum B(GT) up to 40 MeV ~ 0.7-0.8
(Old calculation: 0.66)

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

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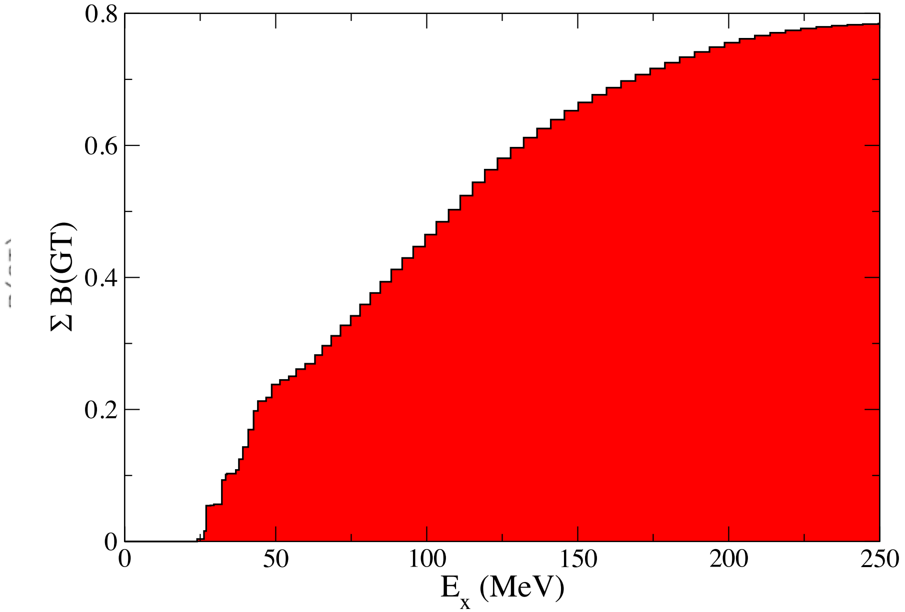

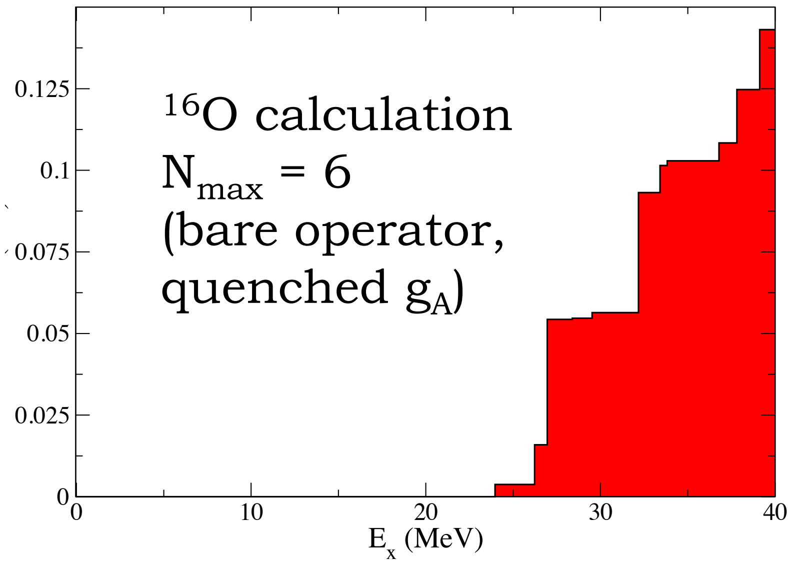

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^{18}F shell model calculations

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It's not clear what effect these correlations will have on PNC matrix elements.

Can test by artificially lowering 4p-4h states in ^{12}C, ^{16}O by adjusting single-particle energies, monopole terms.

Conclusions

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We're in a new 'golden age' of nuclear structure calculations, powered by new techniques and supercomputers!

Can do rigorous *ab initio* calculations of many nuclear properties, especially in the lower *p*-shell.

But additional challenges arise in the upper *p*-shell and lower *sd*-shell, specifically the alpha-particle clusters seen in the Hoyle state and analogs in nearby nuclei.