Implementations of NuShellX

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UNEDF support for three months this summer

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BAB

NuShellX starts with good-J proton and neutron basis states.
Then a good-J pn basis is generated from vector coupling:

$$| \, [(J_p, \alpha_p) \otimes (J_n, \alpha_n)] J >$$

Fortran95
OpenMP
The Hamiltonian matrix is obtained “on the fly”
Windows and Linux

NuShellX@MSU is a set of wrapper codes that makes the program very easy to install and run with standard inputs and outputs.
There are many more options that can be accessed by the expert users. The code is open-source so you can make changes.

The proton and neutron basis states are obtained by angular momentum projection from M states with the underlying code NuShell.

NuShell is a Fortran95 replacement for Oxbash

But the use of NuShell (Oxbash) for mixed proton-neutron States is very limited by the time and space needed for projection and matrix storage. NuShellX solves this problem.

The Hamiltonian is written as a sum of three terms:

$$H = H_{nn} + H_{pp} + H_{pn}$$

The second quantized form for H_{pn} is

$$H_{pn} = \sum_{pnp'n',J_o} < pnJ_o \mid V \mid p'n'J_o > \{[a_p^+ a_n^+]^{J_o} \otimes [\tilde{a}_{p'}\tilde{a}_{n'}]^{J_o}\}^{(0)}$$

We can recouple the operators to:

$$\{[a_p^+ a_n^+]^{J_o} \otimes [\tilde{a}_{p'}\tilde{a}_{n'}]^{J_o}\}^{(0)} = -\sum_{\lambda} \sqrt{(2\lambda+1)(2J_o+1)}\,(-1)^{n+p'-\lambda-J_o} \begin{Bmatrix} p & n & J_o \\ n' & p' & \lambda \end{Bmatrix} \{[a_p^+ \tilde{a}_{p'}]^{\lambda} \otimes [a_n^+ \tilde{a}_{n'}]^{\lambda}\}^{(0)}$$

where, for example, p stands for the single-particle wavefunction (n_p, ℓ_p, j_p) or for just j_p in the six-j or phase factor. H_{pn} can thus be written in the particle-hole form:

$$H_{pn} = \sum_{pp'nn'\lambda} F_\lambda(pp'nn') \; \{[a_p^+ \tilde{a}_{p'}]^\lambda \otimes [a_p^+ \tilde{a}_{n'}]^\lambda\}^{(0)}$$

where

$$F_\lambda(pp'nn') = -\sum_{J_o} \sqrt{(2\lambda+1)(2J+1)}\,(-1)^{n+p'-\lambda-J_o} \left\{ \begin{array}{ccc} p & n & J_o \\ n' & p' & \lambda \end{array} \right\} < pnJ_o \mid V \mid p'n'J_o >$$

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The NuShellX basis states have the form:

$$| B, J >= | [(J_p, \alpha_p) \otimes (J_n, \alpha_n)] J >$$

For the Lanczos multiplications we need the matrix elements:

$$< B_f, J \mid H_{nn} \mid B_i, J >= \delta_{J_{p_f}, J_{p_i}} \delta_{\alpha_{p_f}, \alpha_{p_i}} \delta_{J_{n_f}, J_{n_i}} < (J_{n_f}, \alpha_{n_f}) \mid H_{nn} \mid (J_{n_i}, \alpha_{n_i}) >$$

$$< B_f, J \mid H_{pp} \mid B_i, J >= \delta_{J_{n_f}, J_{n_{2i}}} \delta_{\alpha_{n_f}, \alpha_{n_i}} \delta_{J_{p_f}, J_{p_i}} < (J_{p_f}, \alpha_{p_f}) \mid H_{pp} \mid (J_{p_i}, \alpha_{p_i}) >$$

and

$$< B_f, J \mid H_{pn} \mid B_i, J >= \sum_{pp'nn', l} F_\lambda(pp'nn')$$

$$\times < [(J_{p_f}, \alpha_{p_f}) \otimes (J_{n_f}, \alpha_{n_f})] J \mid \{[a_p^+ \tilde{a}_{p'}]^\lambda \otimes [a_p^+ \tilde{a}_{n'}]^\lambda\}^{(0)} \mid [(J_{p_i}, \alpha_{p_i}) \otimes (J_{n_i}, \alpha_{n_i})] J >$$

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$$< B_f, J \mid H_{pn} \mid B_i, J >= \sum_{pp'nn'\lambda} F_\lambda(pp'nn')\ \Gamma_\lambda\ \mathrm{RDM}(p_f, p_i, p, p', \lambda)\ \mathrm{RDM}(n_f, n_i, n, n', \lambda)$$

where, for example, p_f, stands for labels (J_{p_f}, α_{p_f}),

$$\Gamma_\lambda = \left\{ \begin{array}{ccc} J_{p_f} & J_{p_i} & \lambda \\ J_{n_f} & J_{n_i} & \lambda \\ J & J & 0 \end{array} \right\}$$

and RDM are the reduced density matricies:

$$\mathrm{RDM}(p_f, p_i, p, p', \lambda) = < [(J_{p_f}, \alpha_{p_f})||[a_p^+ \tilde{a}_{p'}]^\lambda||[(J_{p_i}, \alpha_{p_i}) >$$

and

$$\mathrm{RDM}(n_f, n_i, n, n', \lambda) = < [(J_{n_f}, \alpha_{n_f})||[a_n^+ \tilde{a}_{n'}]^\lambda||[(J_{n_i}, \alpha_{n_i}) >$$

The key is to optimize the sums in this equation for OpenMP and/or MPI

NATHAN, E. Caurier, G. Martinez-Pinedo, F. Nowacki, A. Poves, J. Retamosa and A. P. Zuker, Phys. Rev. C **59**, 2033 (1999). link

J. Toivanen, arXiv:nucl-th/061002v1 9 Oct 2006.

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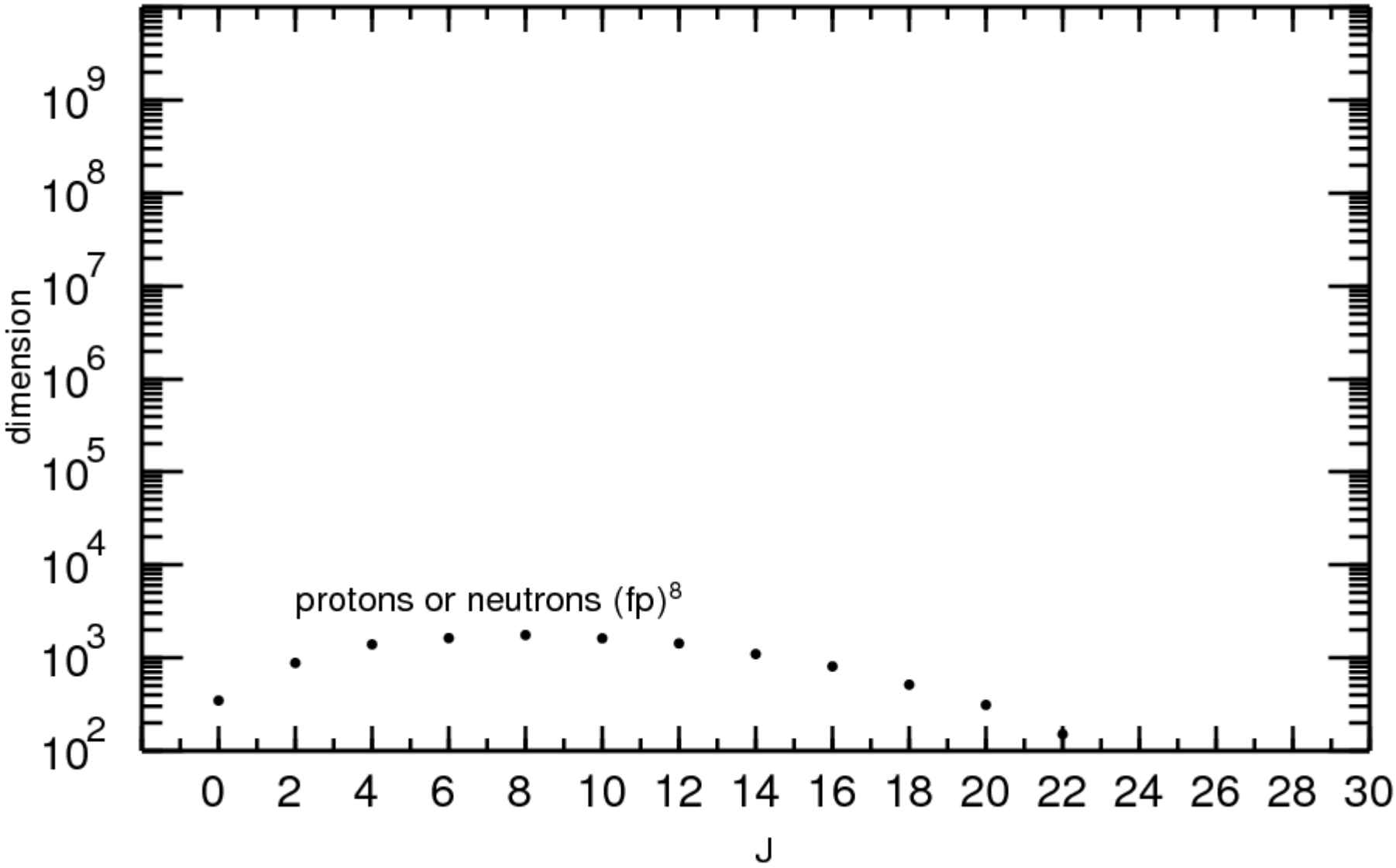
Example for ^{56}Ni in the pf shell



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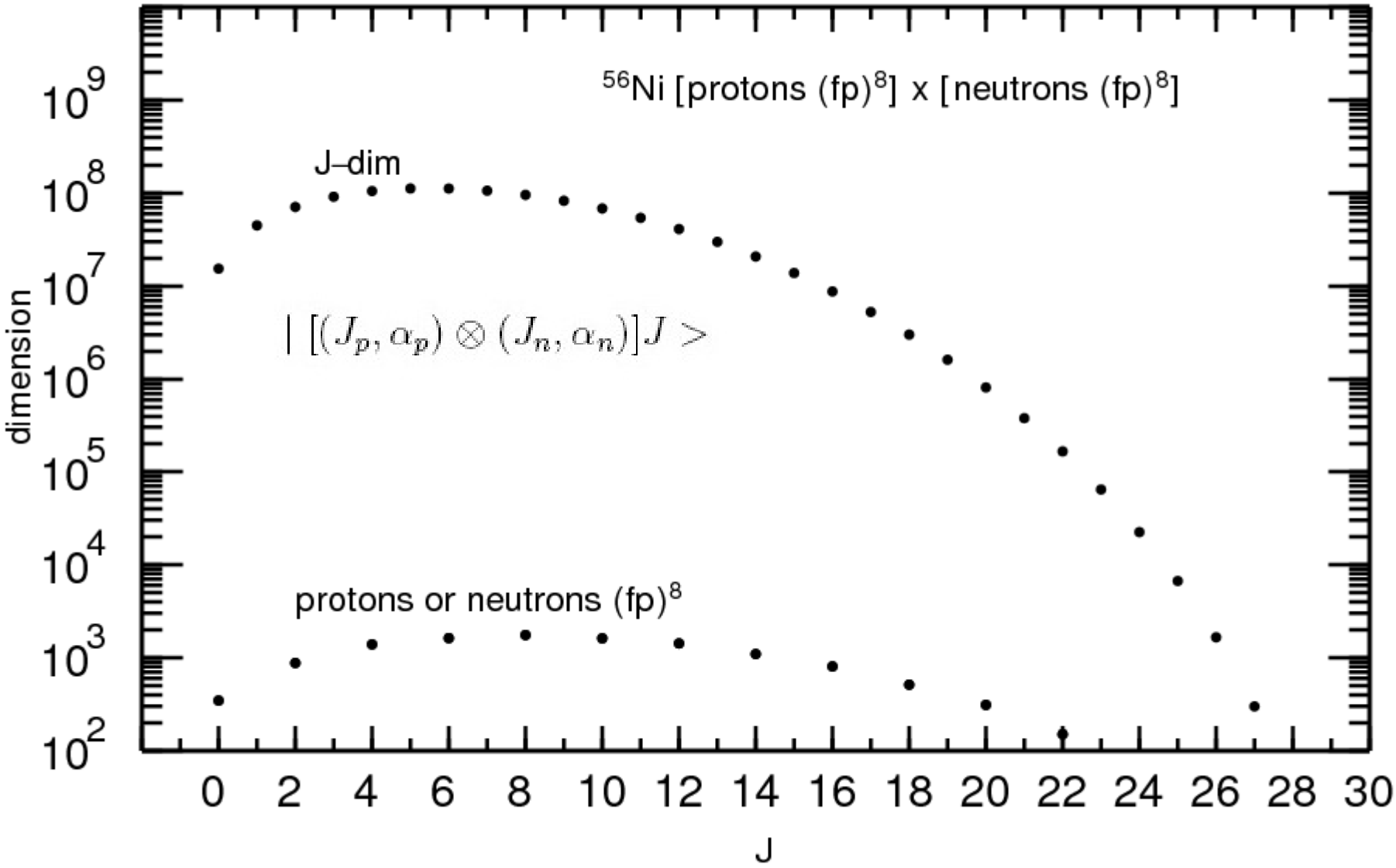

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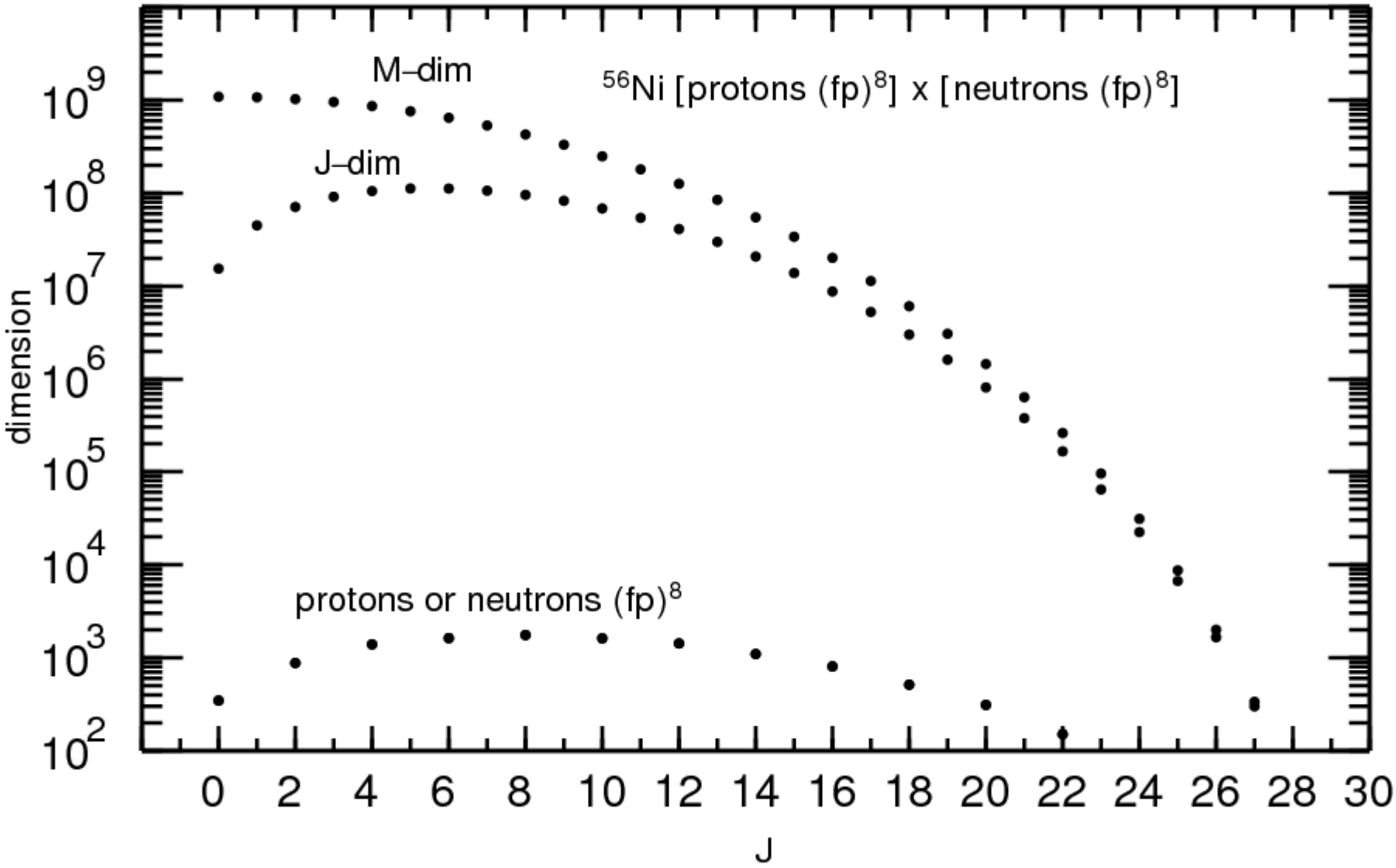

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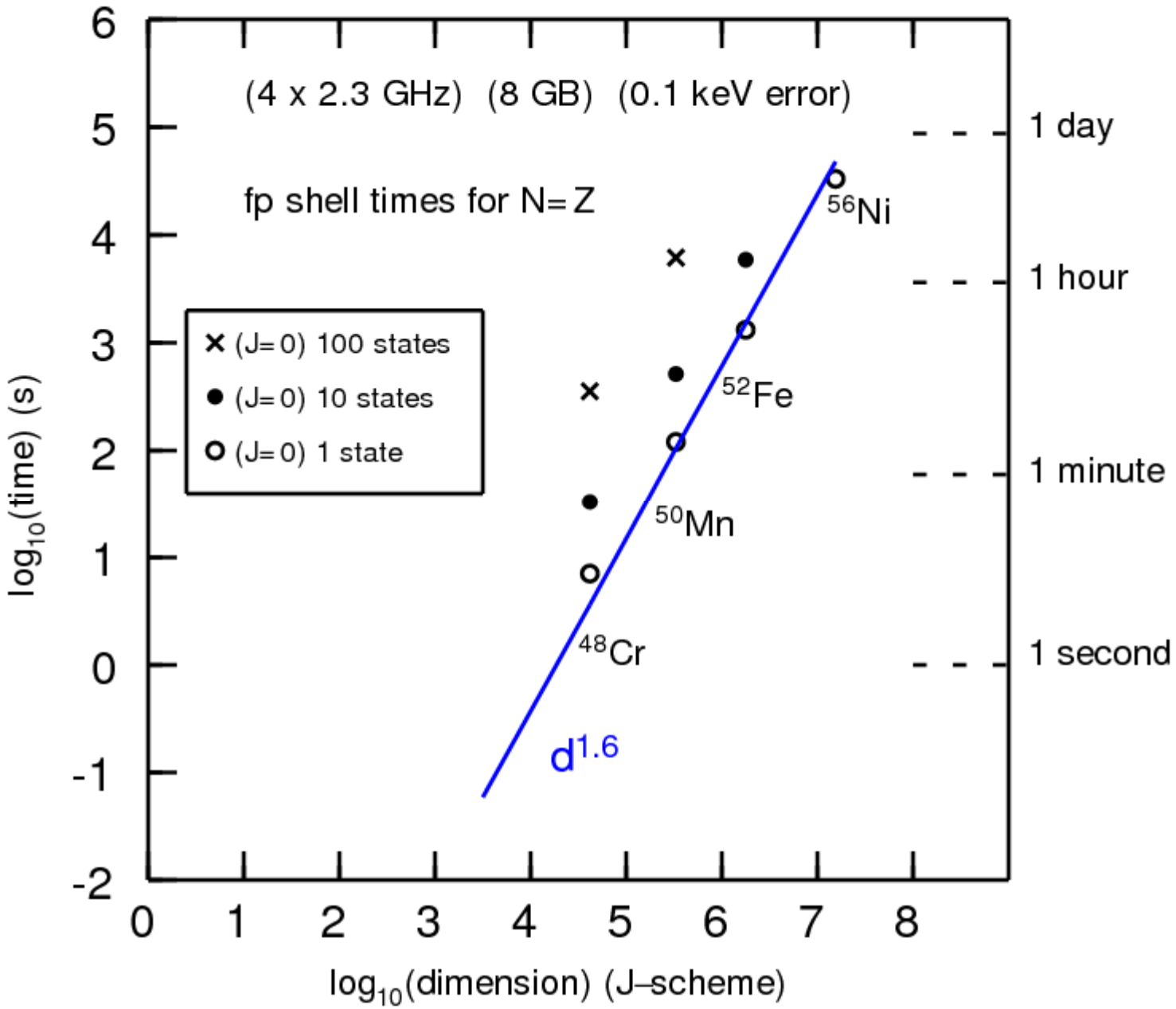

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- Observables
- $< f \mid a^+ \mid i >$ for one-particle spectrosopic factors
- $< f \mid a^+ a \mid i >$ for one-body operators, electromagnetic, beta decay, etc.
- $< f \mid a^+ a^+ \mid i >$ for two-particle spectrosocpic factors
- $< f \mid a^+ a^+ aa \mid i >$ for isospin mixing, parity mixing, etc.

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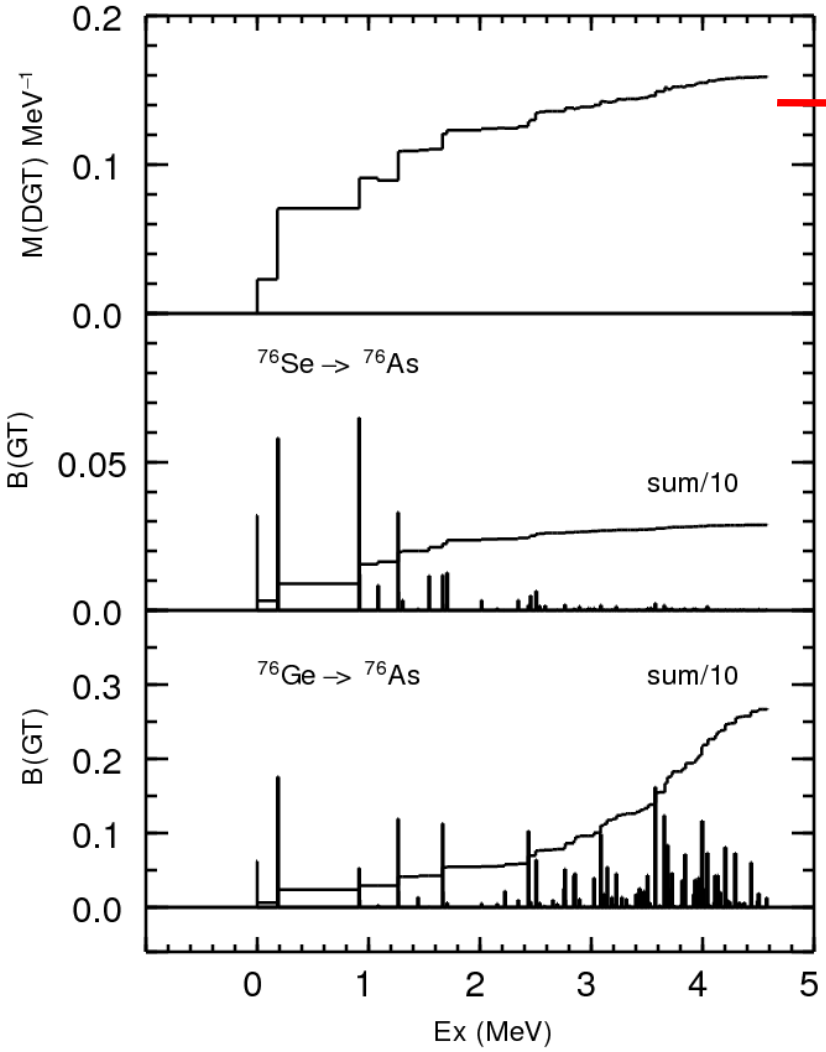
A=76 double-beta calculations based on f5,p3,p1,g9 model space



Value from double-beta experiment

J dimensions on the order of one million
100 J=1 states

(further work needed to evaluate the contributions from f7 and g7)

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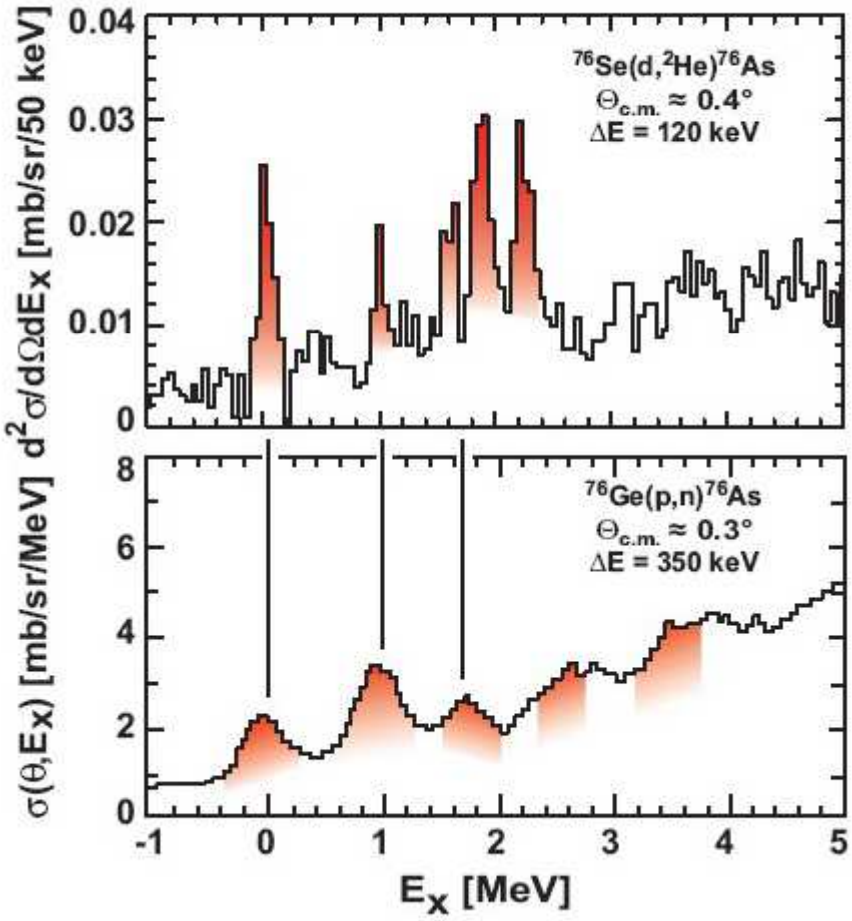
PHYSICAL REVIEW C 78, 044301 (2008)

The $(d, {}^2\mathrm{He})$ reaction on ^{76}Se and the double-β-decay matrix elements for $A = 76$

E.-W. Grewe,[1] C. Bäumer,[1,*] H. Dohmann,[1] D. Frekers,[1] M. N. Harakeh,[2] S. Hollstein,[1] H. Johansson,[3,†] L. Popescu, S. Rakers,[1,§] D. Savran,[2,5] H. Simon,[3] J. H. Thies,[1] A. M. van den Berg,[2] H. J. Wörtche,[2] and A. Zilges[6]



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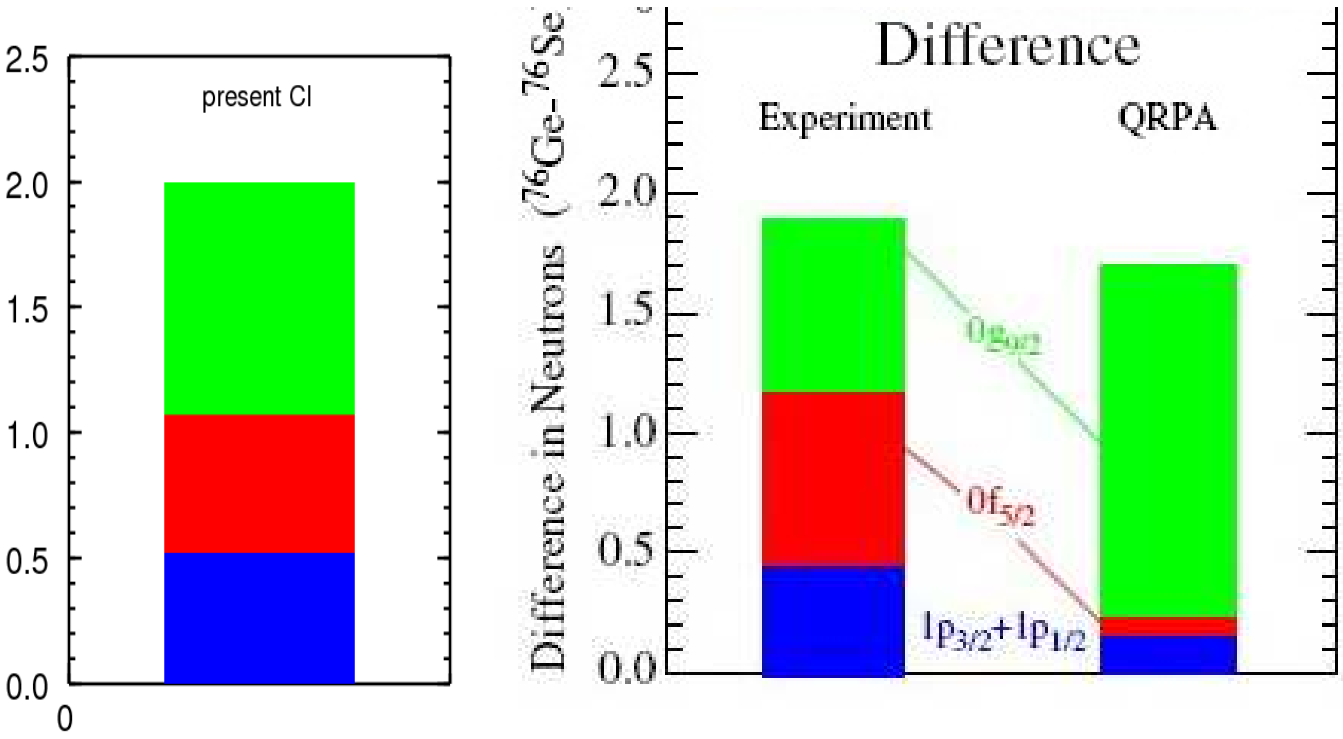
PRL 100, 112501 (2008) PHYSICAL REVIEW LETTERS week ending 21 MARCH 2008

Nuclear Structure Relevant to Neutrinoless Double β Decay: ^{76}Ge and ^{76}Se

J. P. Schiffer,[1,*] S. J. Freeman,[2] J. A. Clark,[3] C. Deibel,[3] C. R. Fitzpatrick,[2] S. Gros,[1] A. Heinz,[3] D. Hirata,[4,5] C. L. Jiang,[1] B. P. Kay,[2] A. Parikh,[3] P. D. Parker,[3] K. E. Rehm,[1] A. C. C. Villari,[4] V. Werner,[3] and C. Wrede[3]



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Truncation based on structure of the basis states

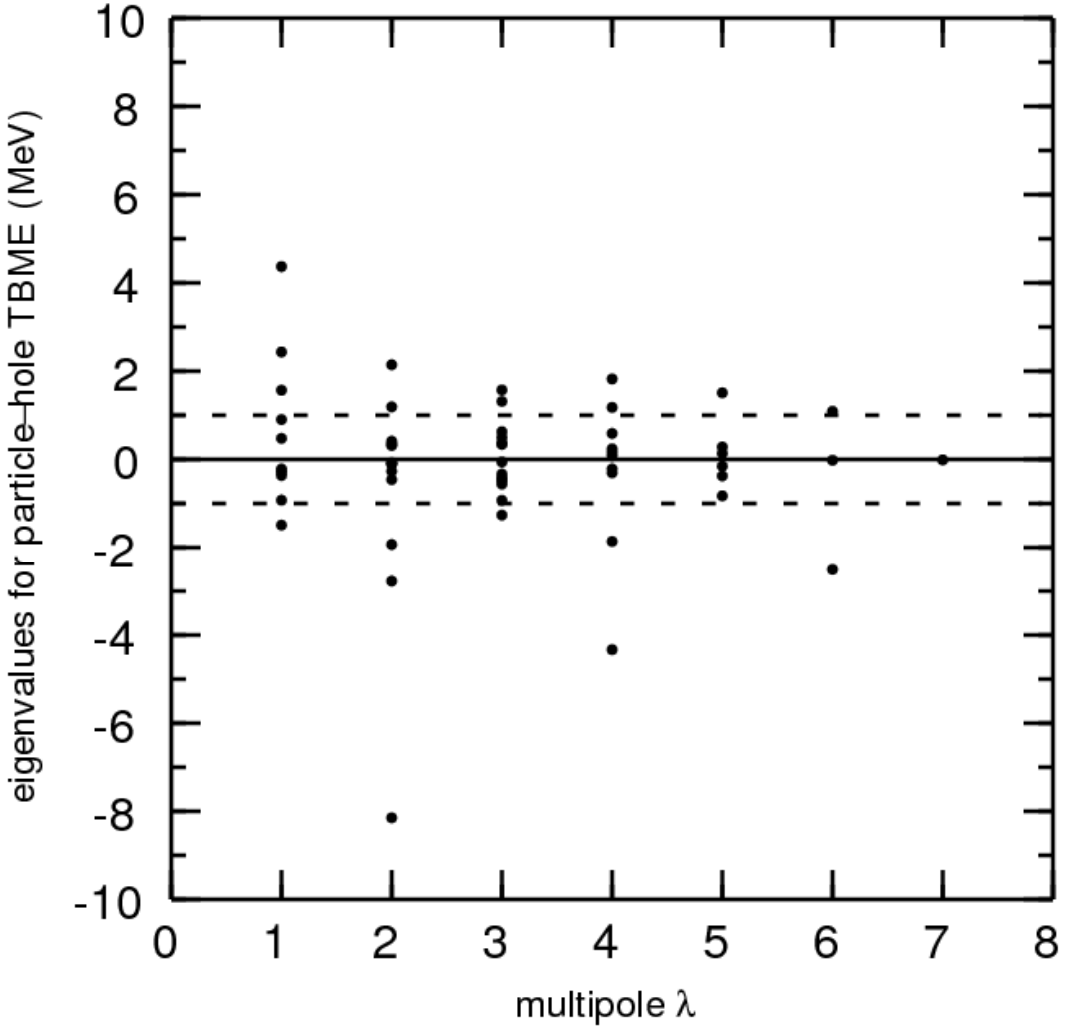
1) proton (neutron) orbital occupations
2) J_p (J_n) of the proton (neutron) basis states
3) eigenvalues of the pn particle-hole TBME

$$H_{pn} = \sum_{pp'nn'\lambda} F_\lambda(pp'nn') \; \{[a_p^+ \tilde{a}_{p'}]^\lambda \otimes [a_p^+ \tilde{a}_{n'}]^\lambda\}^{(0)}$$

where

$$F_\lambda(pp'nn') = -\sum_{J_o} \sqrt{(2\lambda+1)(2J+1)}\,(-1)^{n+p'-\lambda-J_o} \left\{ \begin{array}{ccc} p & n & J_o \\ n' & p' & \lambda \end{array} \right\} < pnJ_o \mid V \mid p'n'J_o >$$

Truncation based on eigenvalues of the particle-hole TBME



Implementation of ideas given in
DuFour and Zuker, PRC54, 1641 (1996)

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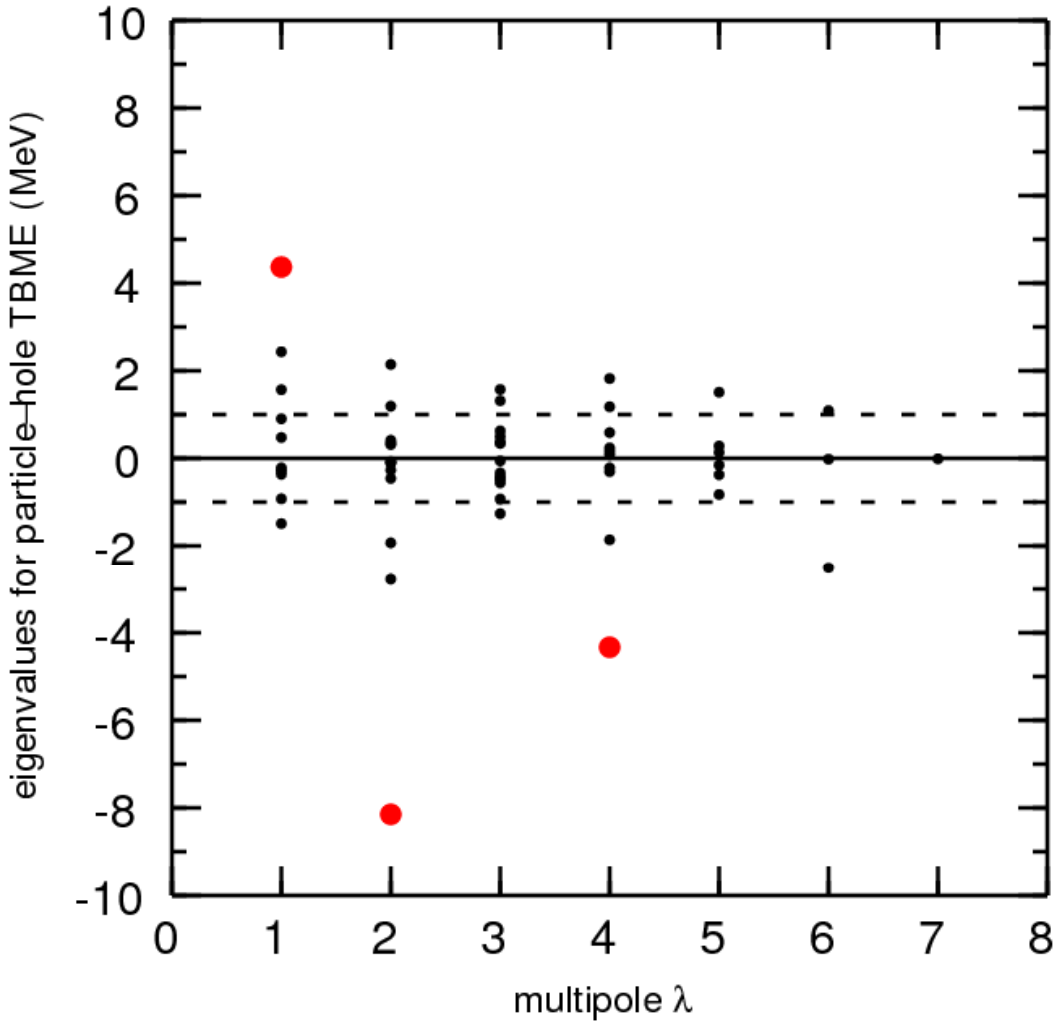
Truncation based on eigenvalues of the particle-hole TBME



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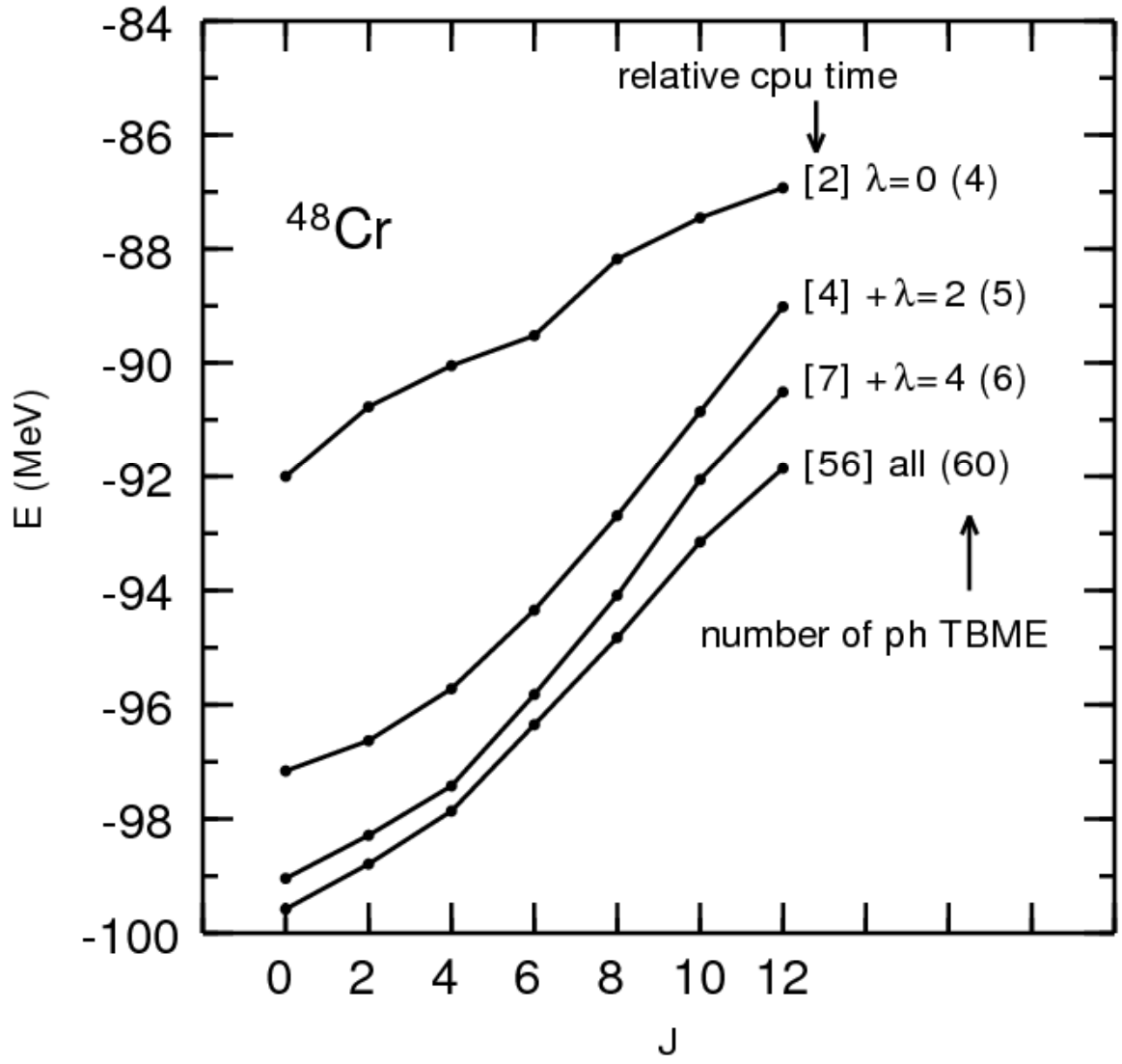
Truncation based on eigenvalues of the particle-hole TBME



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UNEDF - status

OpenMP – speedup is 90% efficient for up to 8 cores.
Speedup saturation is about 40 (compared to one core)

Since matrix is not needed, storage is relatively small
- e.g. 10s of GB for 100,000,000 J (10 billion M) states.

Summer project with Lisetskiy
- What are the limiting factors?
- How to make NuShellX more efficient?
- Try MPI – i.e., Cluster-OpenMP

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UNEDF - future plans (year 4-5)

Computation: details depend on results of this summer.

With the code now
- each J is independent (e.g. 10 per nucleus)
- each nucleus is independent

e.g. one pass for the A=56-100 mass region could involve about
(one J) x (number of J) x (number of nuclei)
= 64 x 10 x 80 = 50,000 cores (with about 50% efficiency)

We need to find good Hamiltonians for the A=56-100 mass region

Transformational applications up to ^{100}Sn
- Double-beta decay for A=76 and A=82
- Understanding the nuclear rapid-proton-capture-process
- Fermi decay for extracting v_{ud}

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