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Stronger nuclear structure calculations for weak physics

Calvin W. Johnson

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Searching for ν physics, LBL, Jan 8, 2020

An all-too-common view:

An all-too-common view:

Dark matter, string theory, neutrino physics….

An all-too-common view:

Dark matter, string theory, neutrino physics….

Nuclear structure physics

An all-too-common view:

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Dark matter, string theory, neutrino physics….

Nuclear structure physics

A better view:

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Dark matter, string theory, neutrino physics….

Nuclear structure physics

A better view:

Modern nuclear structure physics is rigorous, vigorous, and *the launchpoint for many other investigations.*

Our story so far….

We have made great strides in *ab initio* calculations of nuclear structure, e.g.,

the *no-core shell model* (NCSM), using

interactions fit to NN data, for example,

- The HOBET project (talks by Tom Luu, Ken McElvain)
- χEFT
- etc

Good primarily for light nuclei, though can extend via in-medium similarity renormalization group (IM-SRG)

Our story so far….

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But many applications often require matrix elements in heavy nuclei:

- dark matter cross sections (Xe, Ge, etc.)
- parity-violating "anapole" moment in cesium and similar nuclei
- measurement of permanent electric dipole moments in ^{199}Hg (Schiff moment)
- and of course, neutrinoless double-beta decay

Our story so far….

But many applications often require

matrix

- dark … Ge, etc.)
- pari… in cesium
  a…
- n… ic dipo
  n… ment)
- a… ouble-beta d

Many of these targets are so heavy, difficult to reach by conventional shell model

The goal of reaching heavy nuclei by configuration-interaction inspired this talk

To compute transition rates, we use Fermi's (actually Dirac's) Golden Rule from time-dependent perturbation theory:

$$R_{i \to f} = \frac{2\pi}{\hbar} \left| \langle f | \hat{O} | i \rangle \right|^2 \frac{dN_f}{dE}$$

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Transition probability (strength)

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$$R_{i \to f} = \frac{2\pi}{\hbar} \left| \langle f | \hat{O} | i \rangle \right|^2 \frac{dN_f}{dE}$$

Transition probability (strength)

Now you need to compute the transition strength!

To get the many-body states, we use the matrix formalism (a.k.a *configuration-interaction)*

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

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

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

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State of the art shell model calculations late 1980's

dim 386,000 ^{16}O 4p-4h

VOLUME 65, NUMBER 11 PHYSICAL REVIEW LETTERS 10 SEPTEMBER 1990

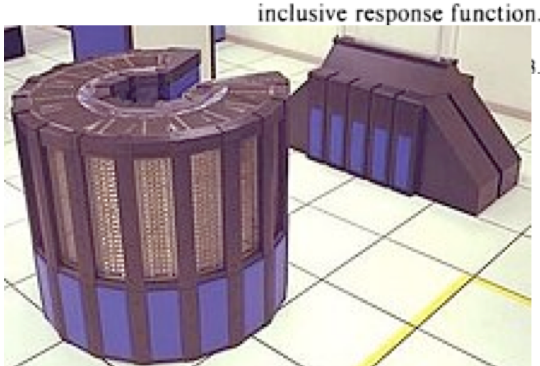
Weak-Interaction Rates in ^{16}O

W. C. Haxton
Department of Physics, FM-15, University of Washington, Seattle, Washington 98195

Calvin Johnson
W. K. Kellogg Radiation Laboratory, California Institute of Technology, Pasadena, California 91125

(Received 29 May 1990)

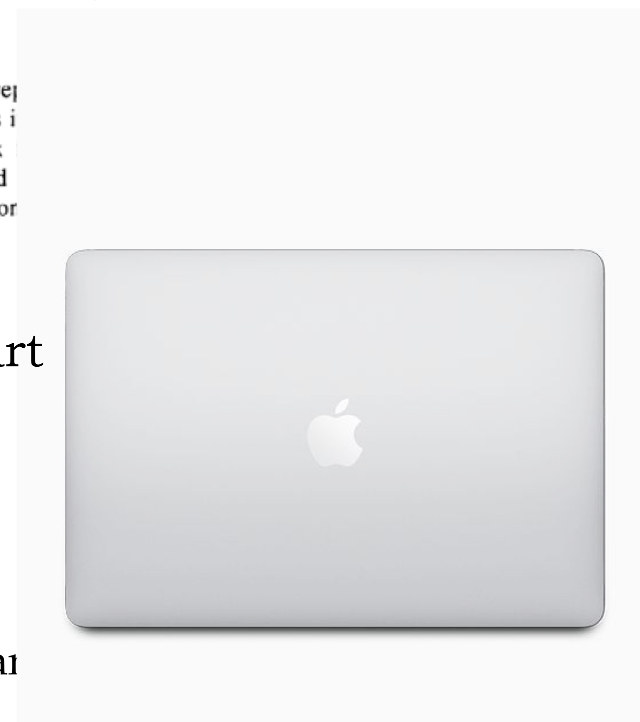
We describe a full nonspurious $4\hbar\omega$ shell-model calculation that successfully re
spectrum of ^{16}O, including the superdeformed 0^+ (6.05 MeV) state, and discuss i
coexistence model. This treatment provides a realistic microscopic framework
electroweak processes: $E2$ transitions in ^{16}O, the role of exchange currents and
pling constant in the $0^+ \leftrightarrow 0^-$ β-decay and μ-capture transition, and the evaluatior
inclusive response function.



.40.−s. 25.30.−c. 27.20.+n

A Cray-2, state of the art in 1985

Now in museums!



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Despite advances, it is easy to get to model spaces beyond our reach:

sd shell: max dimension 93,000. *Can be done in a few minutes on a laptop.*

pf shell: ^{48}Cr, dim 2 million, ~10 minutes on laptop
^{52}Fe, dim 110 million, a few hours on modest workstation
^{56}Ni, dim 1 billion, 1 day on advanced workstation
^{60}Zn, dim 2 billion, < 1 hour on supercomputer

Despite advances, it is easy to get to model spaces beyond our reach:

shells between 50 and 82 ($0g_{7/2}$ 2s1d $0h_{11/2}$)

^{128}Te: dim 13 million (laptop)

^{127}I: dim 1.3 billion (small supercomputer)

^{128}Xe: dim 9.3 billion (supercomputer)

^{129}Cs: dim 50 billion (haven't tried!)

Can we come up with an alternate approach?

How most shell-model codes represent the basis:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_{\mu}\right\rangle \left|n_{\nu}\right\rangle$$

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How most shell-model codes represent the basis: Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

`BIGSTICK*` is an M-scheme code, meaning total J_z fixed

We have a constraint: $M_p+M_n = M$

*github.com/cwjsdsu/BigstickPublick/   see also   arXiv:1801:08432

How most shell-model codes represent the basis:
Proton-neutron factorization

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BIGSTICK is an M-scheme code, meaning total J_z fixed

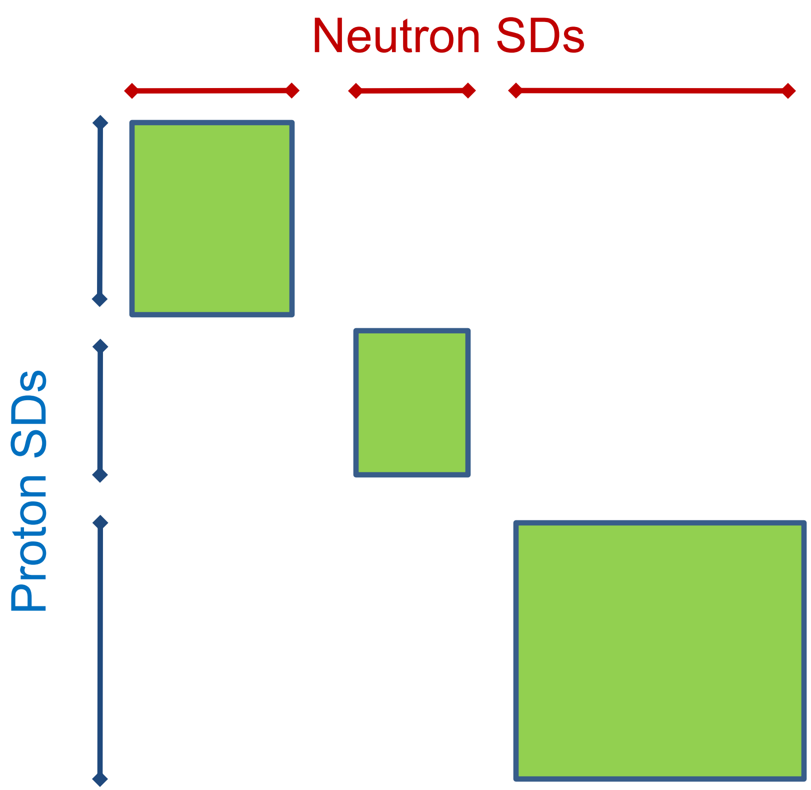
We have a constraint: $M_p + M_n = M$

$$\left|\Psi, M\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_{\mu}, M_{p}\right\rangle \left|n_{\nu}, M_{n} = M - M_{p}\right\rangle$$

Factorization

This leads to a block structure for construction of the basis

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



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

For fast calculation these are typically bit strings, or "*occupation representation of Slater determinants*"

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$\left|01101000...\right\rangle \left|10010100...\right\rangle$$

Alternate approach for medium/nuclei:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Can we truncate for just a few components?

Priori work by Papenbrock, Juodagalvis, Dean, Phys. Rev. C **69**, 024312 (2004), but focused on N =Z

(Also others…)

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Alternate approach for medium/nuclei:
Proton-neutron factorization

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$\left(a_1\left|010110...\right\rangle + a_2\left|110010...\right\rangle + a_3\left|001011...\right\rangle + ...\right)$$

No longer single "Slater determinants" but linear combinations…

Example application:

^{129}Cs: M-scheme dim 50 billion (haven't tried!)

Proton dimension: 14,677
Neutron dimension: 646,430

The idea is to solve proton and neutron problems separately and then couple together a few "select" states

E

1 … en't

Neutron dimension: [illegible],430

Sometimes this is called the 'weak coupling' approximation!

The idea is to solve proton and neutron problems separately and then couple together a few "select" states

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Can the wave function be well-approximated by just a few select proton and neutron states?

These would not be single Slater determinants but linear combinations

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My tool for investigation:
The *entanglement entropy* (See Amol Patwardhan's talk)

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Let any wavefunction have two components (i.e., proton and neutron components)
= "*bipartite*"

Find the singular-value-decomposition eigenvalues of $c_{\mu\nu}$ -- a basis independent characterization of the coupling

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My tool for investigation:
The *entanglement entropy*

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

Note these are proton and neutron many-body states (linear combinations of Slater determinants)

Find the singular-value-decomposition eigenvalues of $c_{\mu\nu}$:

(not the usual density matrix)

Find eigenvalues λ_i of $\rho_{\mu\mu'} = \sum_{\nu} c_{\mu\nu} c_{\mu'\nu}$

$$S = -\sum_i \lambda_i \ln \lambda_i = -tr\,\rho \ln \rho$$

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The *entanglement entropy*

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu\right\rangle \left|n_\nu\right\rangle$$

$$S = -\sum_i \lambda_i \ln \lambda_i = -tr\,\rho \ln \rho$$

The *entanglement entropy* measures how correlated ('entangled') the two sectors are. S=0 means uncorrelated.

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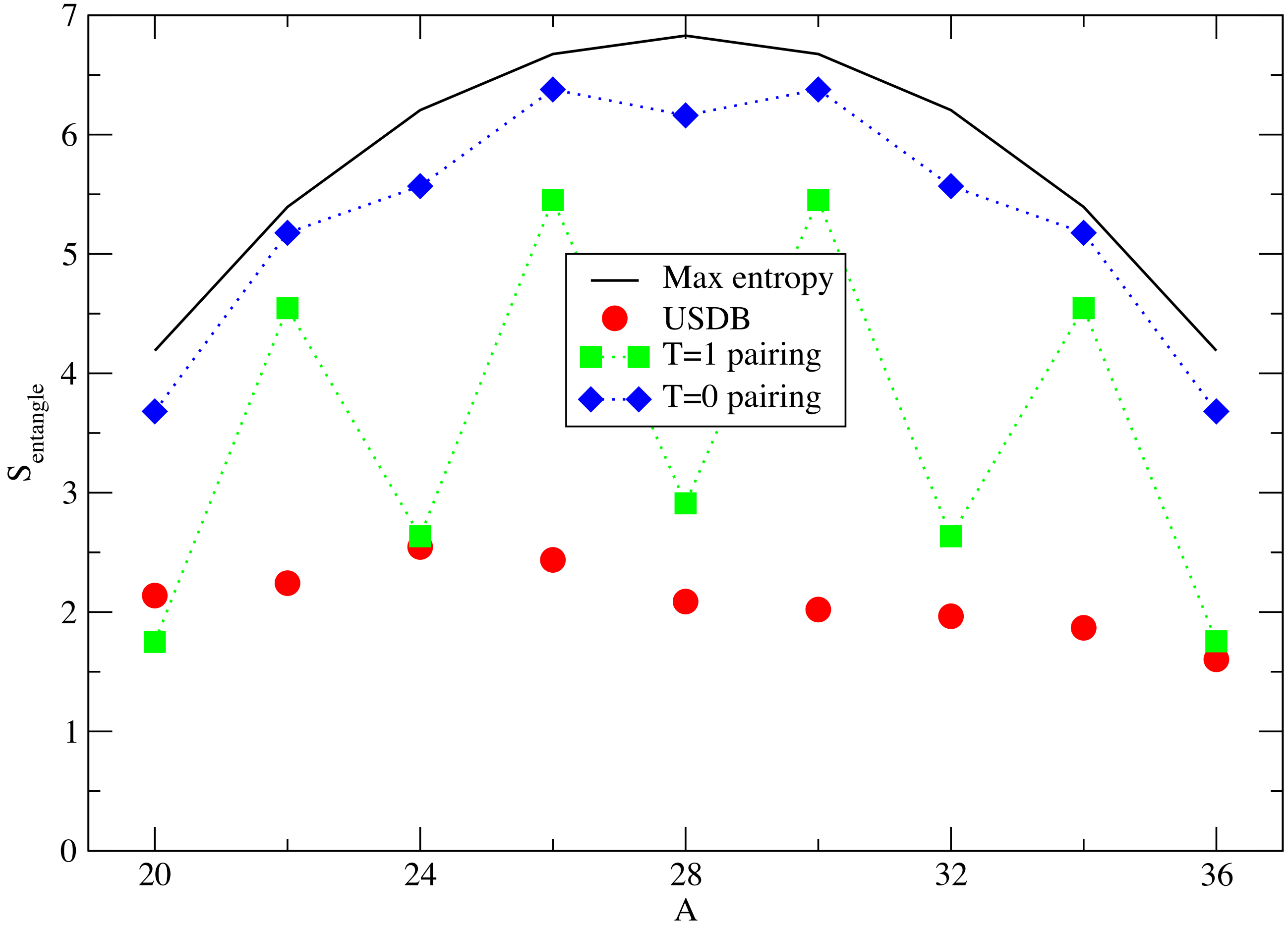
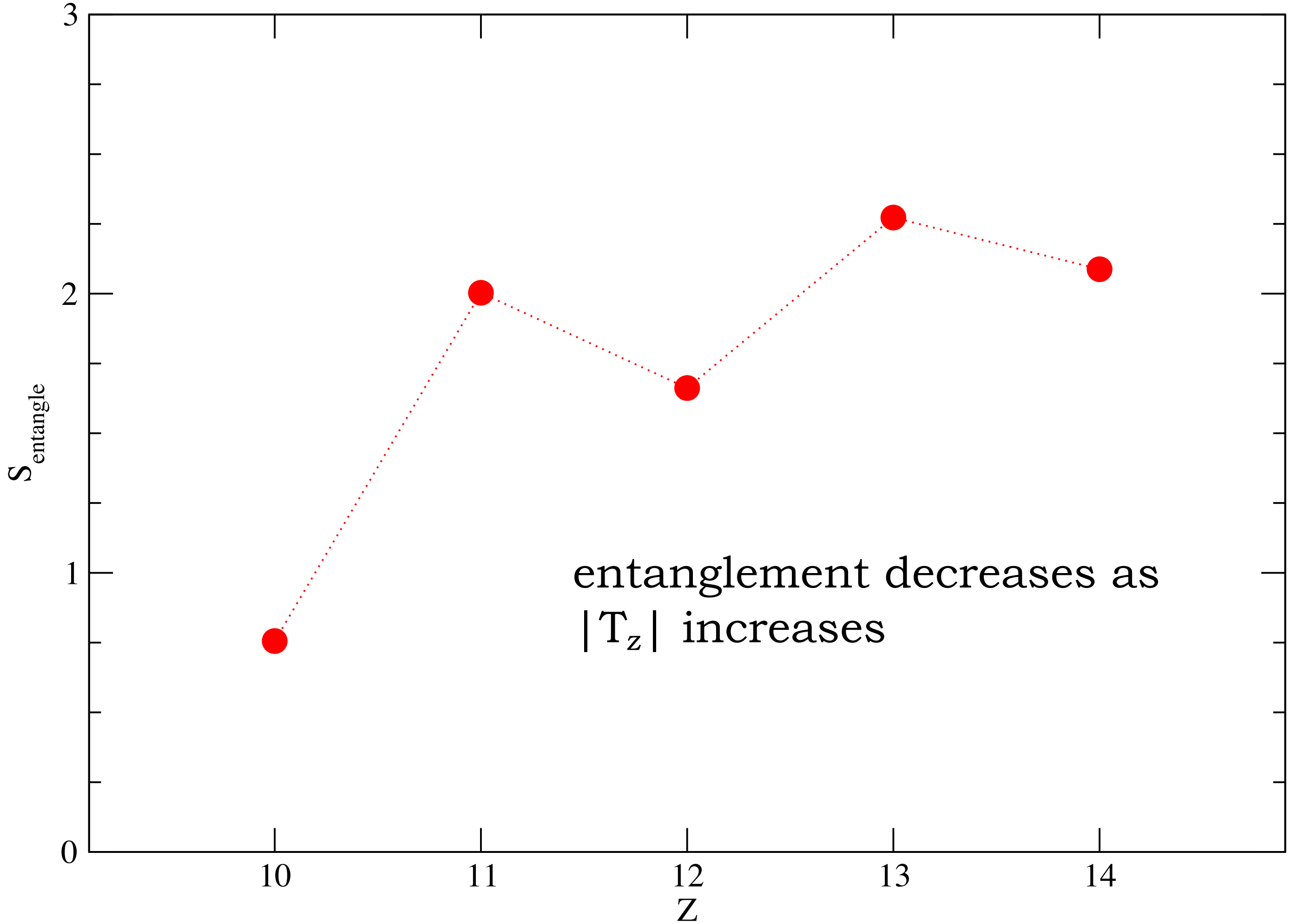
Now let's turn to nuclei, with

$$\left|\Psi\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_{\mu}\right\rangle \left|n_{\nu}\right\rangle$$

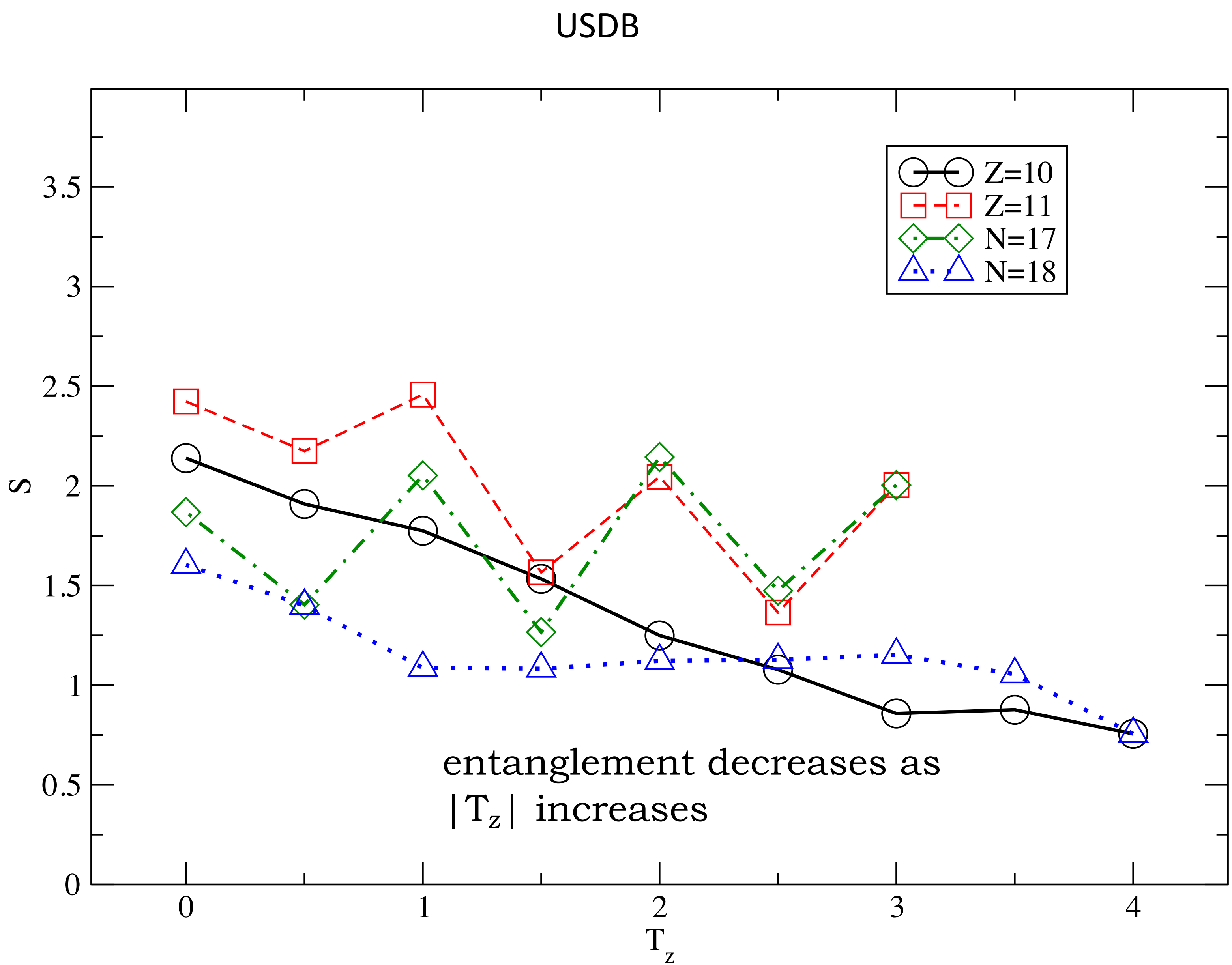


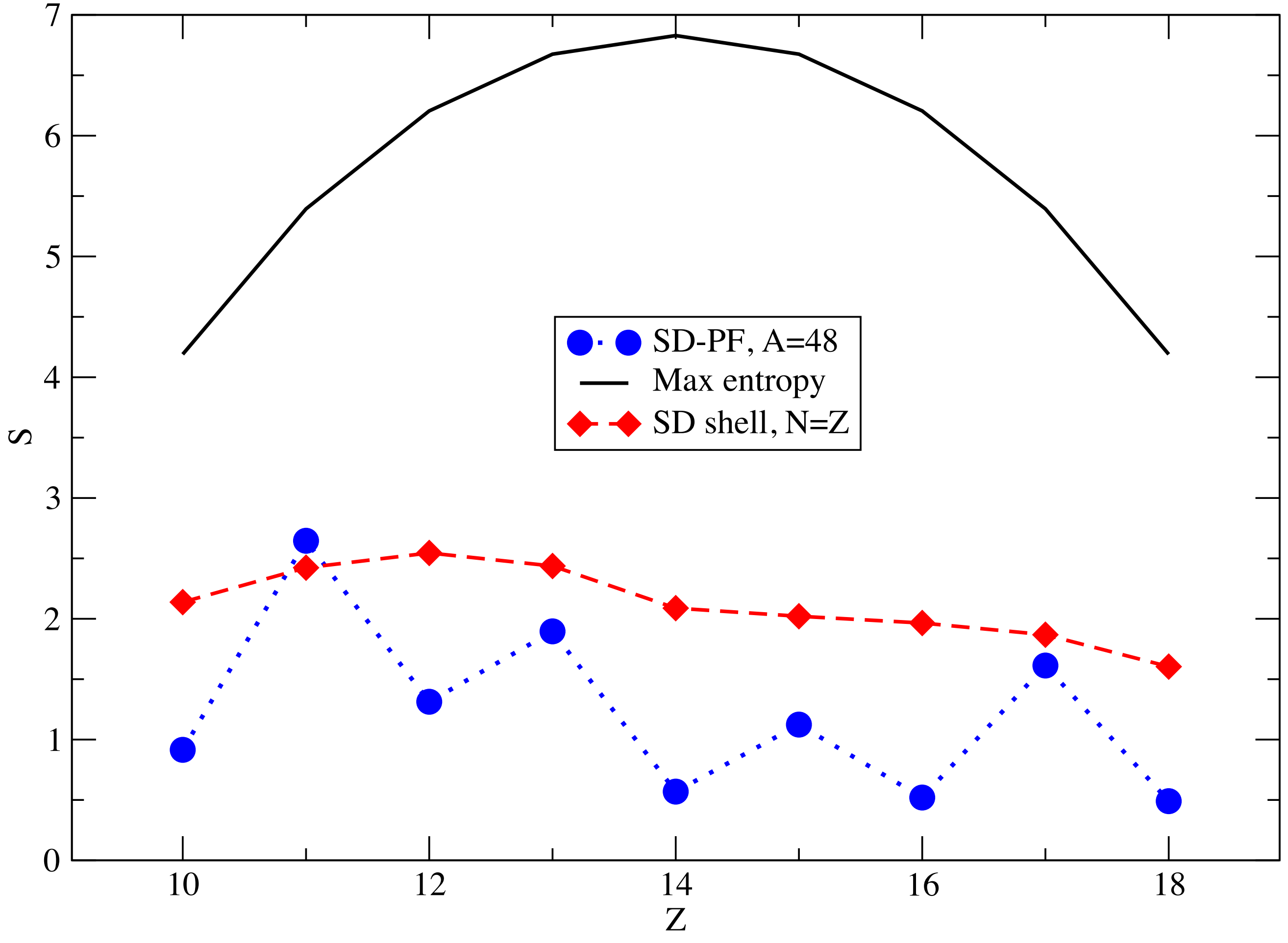
Z=N nuclei
in *sd* shell

Now let's follow
as isospin increases

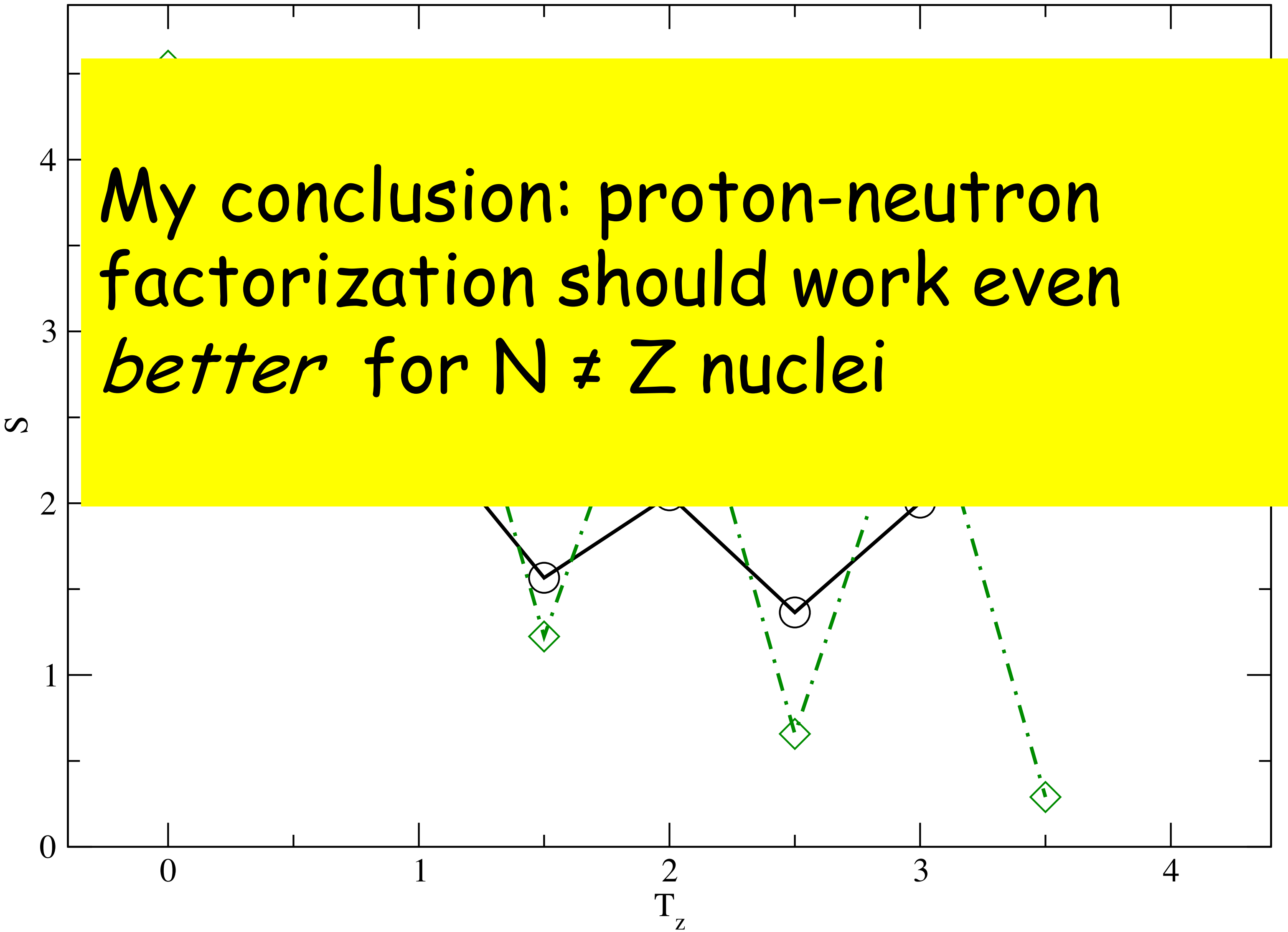


A=28 nuclei
in *sd* shell
with USDB


USDB
Z=10
Z=11
N=17
N=18
S
T_z
entanglement decreases as
$|T_z|$ increases
0
0.5
1
1.5
2
2.5
3
3.5
0
1
2
3
4



Protons *sd*
Neutrons *pf*
(Toy model of heavy nuclie)



My conclusion: proton-neutron factorization should work even *better* for $N \neq Z$ nuclei

PNISM = *proton-neutron interacting shell model*

We have written a code to take advantage of this (O. Gorton)

We want to find solutions to

$$\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle \quad \text{where} \quad \hat{H} = \hat{H}_{pp} + \hat{H}_{nn} + \hat{H}_{p}$$

We solve $\hat{H}_{pp}\left|\Psi_{p}\right\rangle = E_{p}\left|\Psi_{p}\right\rangle \qquad \hat{H}_{nn}\left|\Psi_{n}\right\rangle = E_{n}\left|\Psi_{n}\right\rangle$

and choose certain $\left|\Psi_{p}\right\rangle\left|\Psi_{n}\right\rangle$ as basis for diagonalization;

our results with the entropy suggest we only need a few

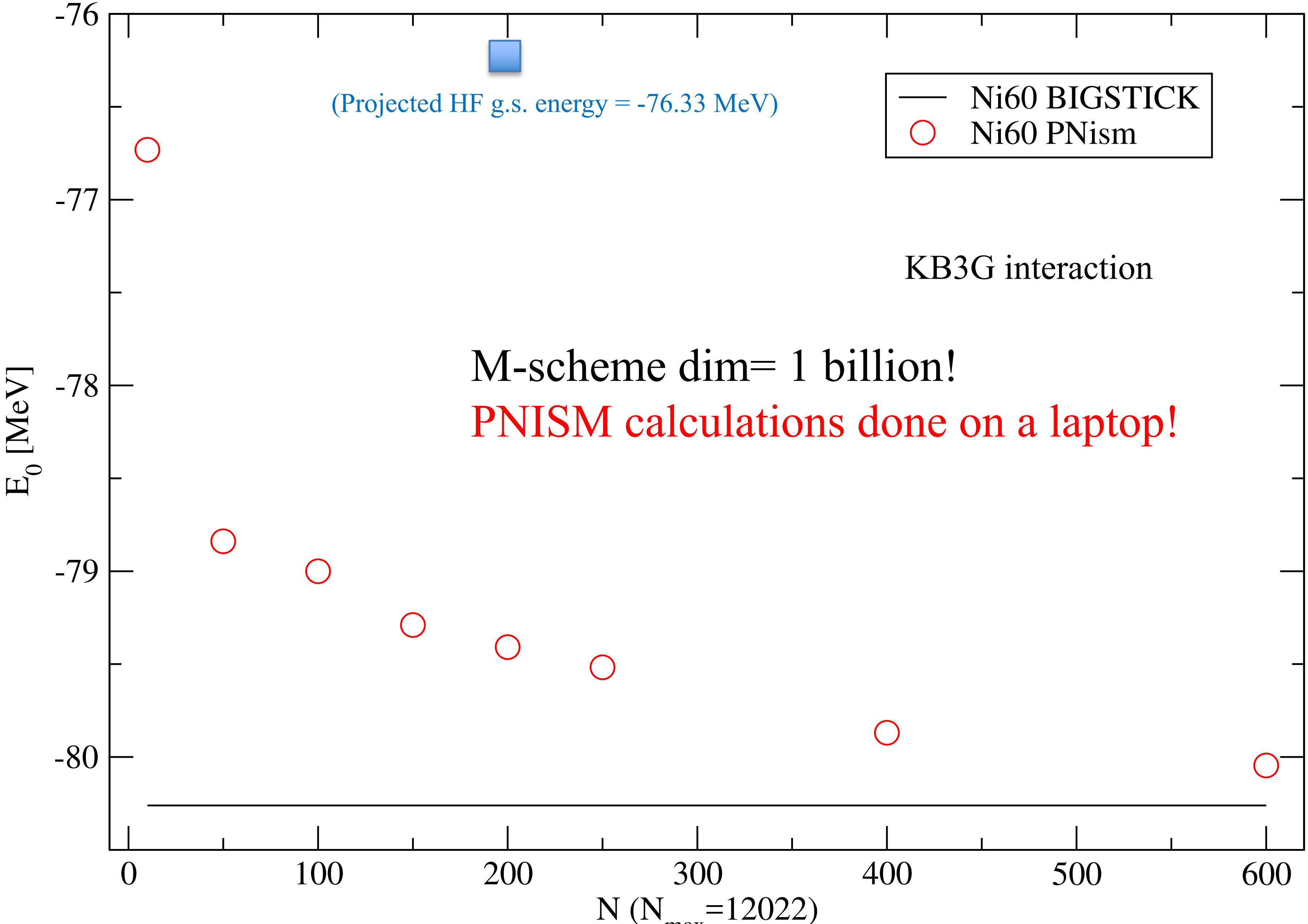
Using BIGSTICK we construct many-proton states of good J

$$\left|\Psi_p, J_p M\right\rangle = \sum_{\mu} c_{\mu} \left|p_{\mu}, M\right\rangle$$

and the same for many-neutron states; these we couple together in a *J-scheme* code with fixed *J* for basis:

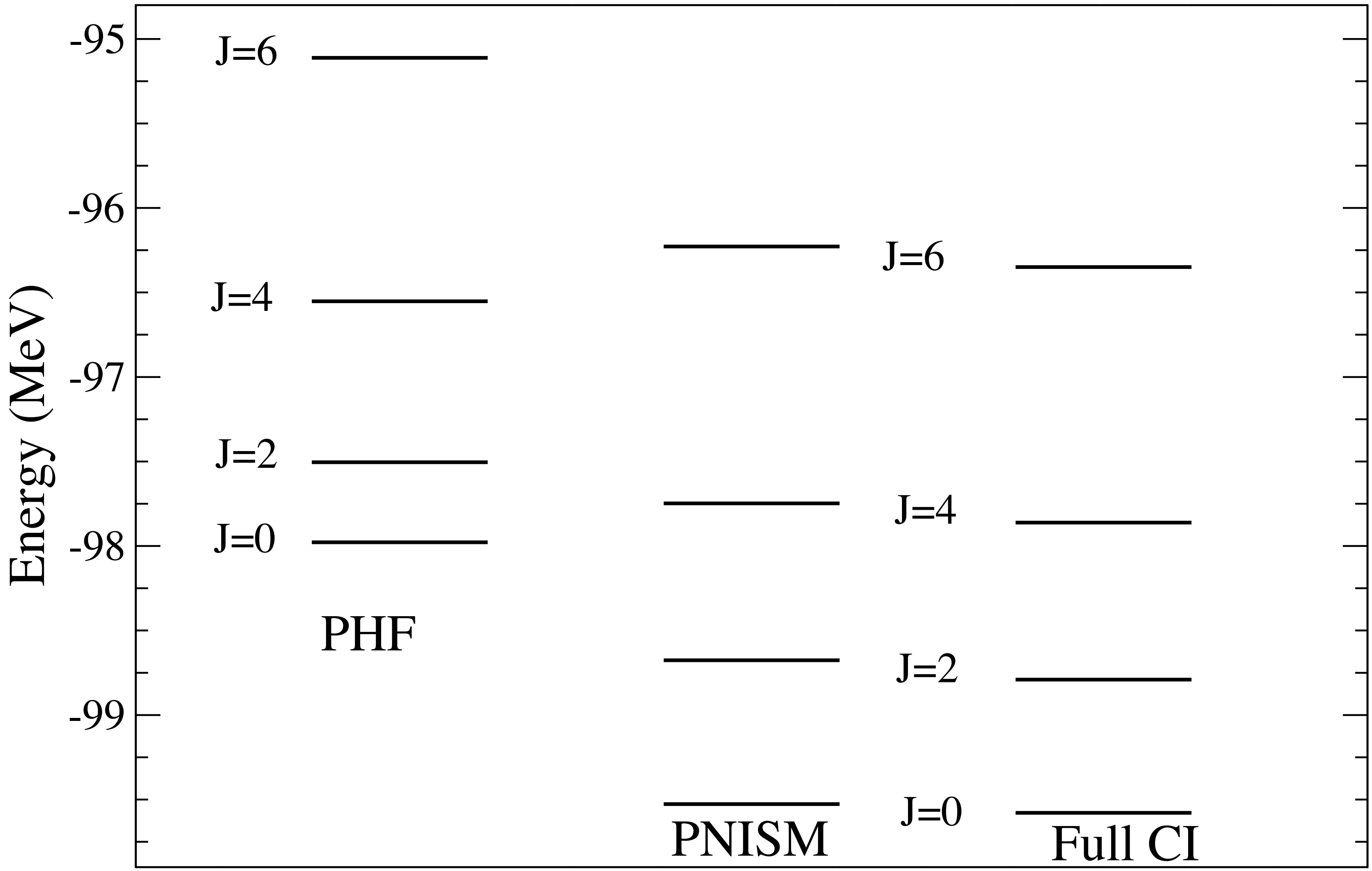
$$\left|\Psi_J\right\rangle = \sum_{ab} c_{ab} \left[\left|\Psi_p a, J_p\right\rangle \otimes \left|\Psi_n b, J_n\right\rangle\right]_J$$

we find matrix elements of the Hamiltonian in basis of these states and diagonalize.



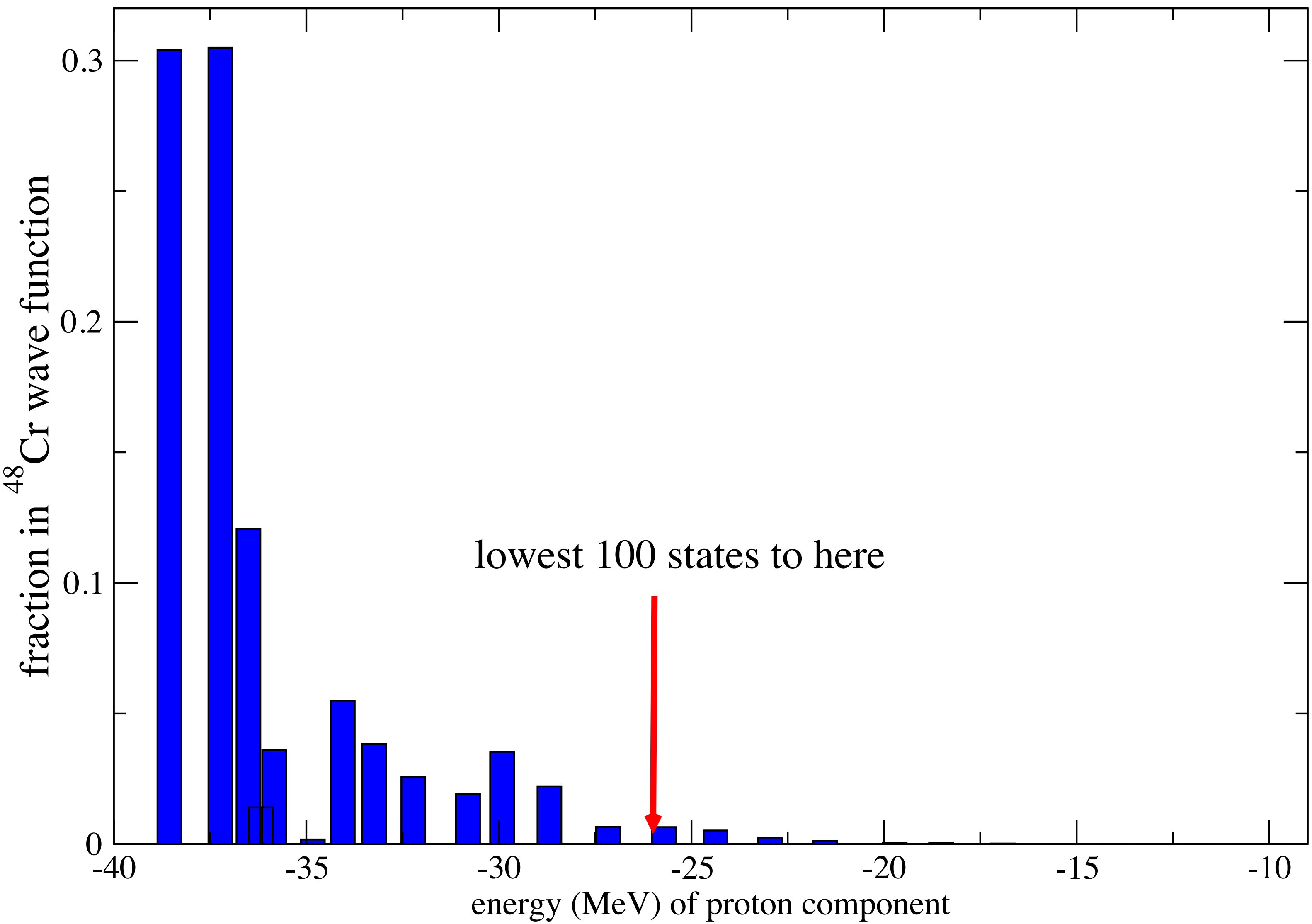
-76
-77
-78
-79
-80
E0 [MeV]
0
100
200
300
400
500
600
N (Nmax=12022)
(Projected HF g.s. energy = -76.33 MeV)
Ni60 BIGSTICK
Ni60 PNism
KB3G interaction
M-scheme dim= 1 billion!
PNISM calculations done on a laptop!

^{48}Cr, GX1A interaction

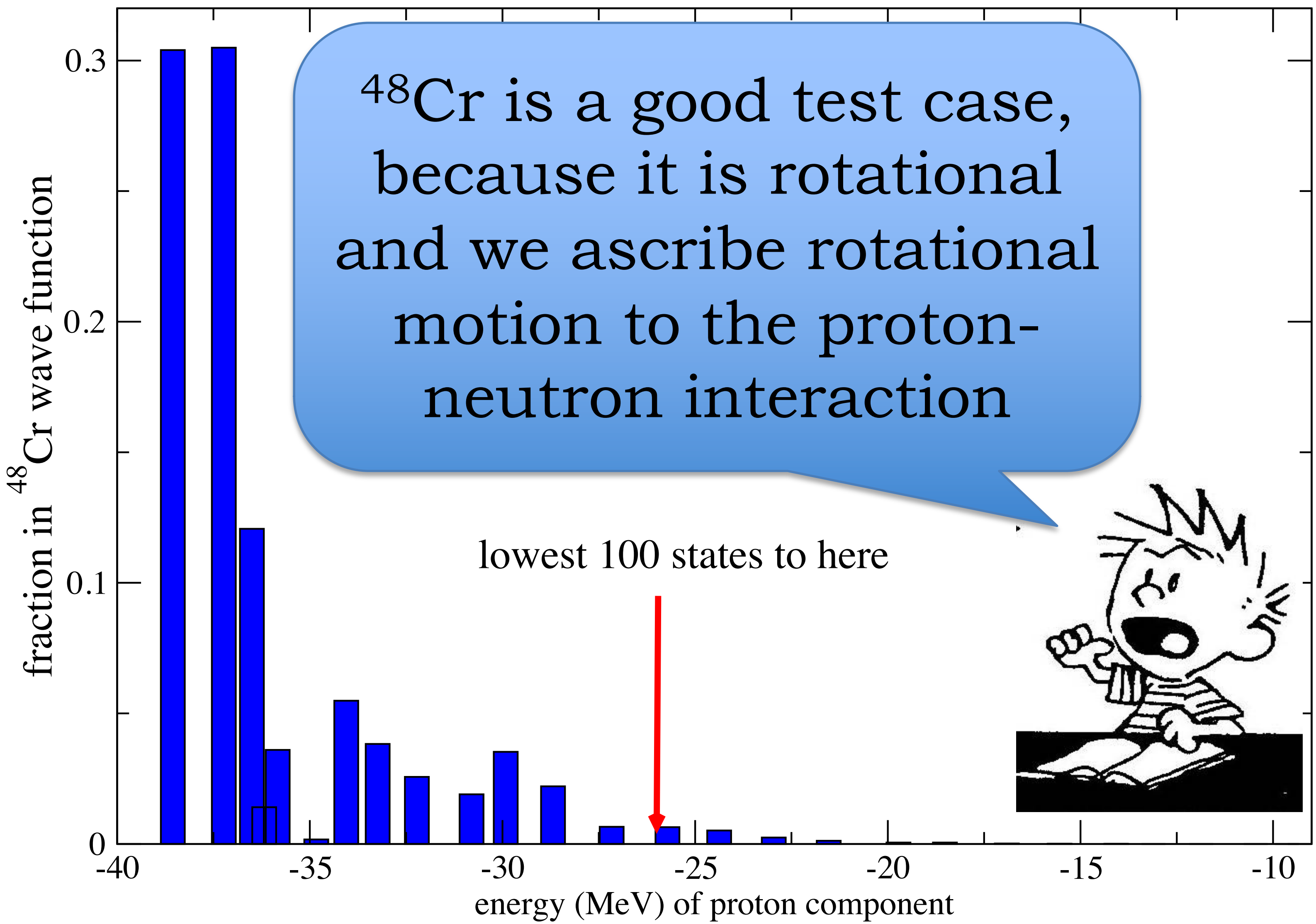


PNISM used 250 proton and 250 neutron levels (out of 4845 each)

^{48}Cr, GX1A interaction

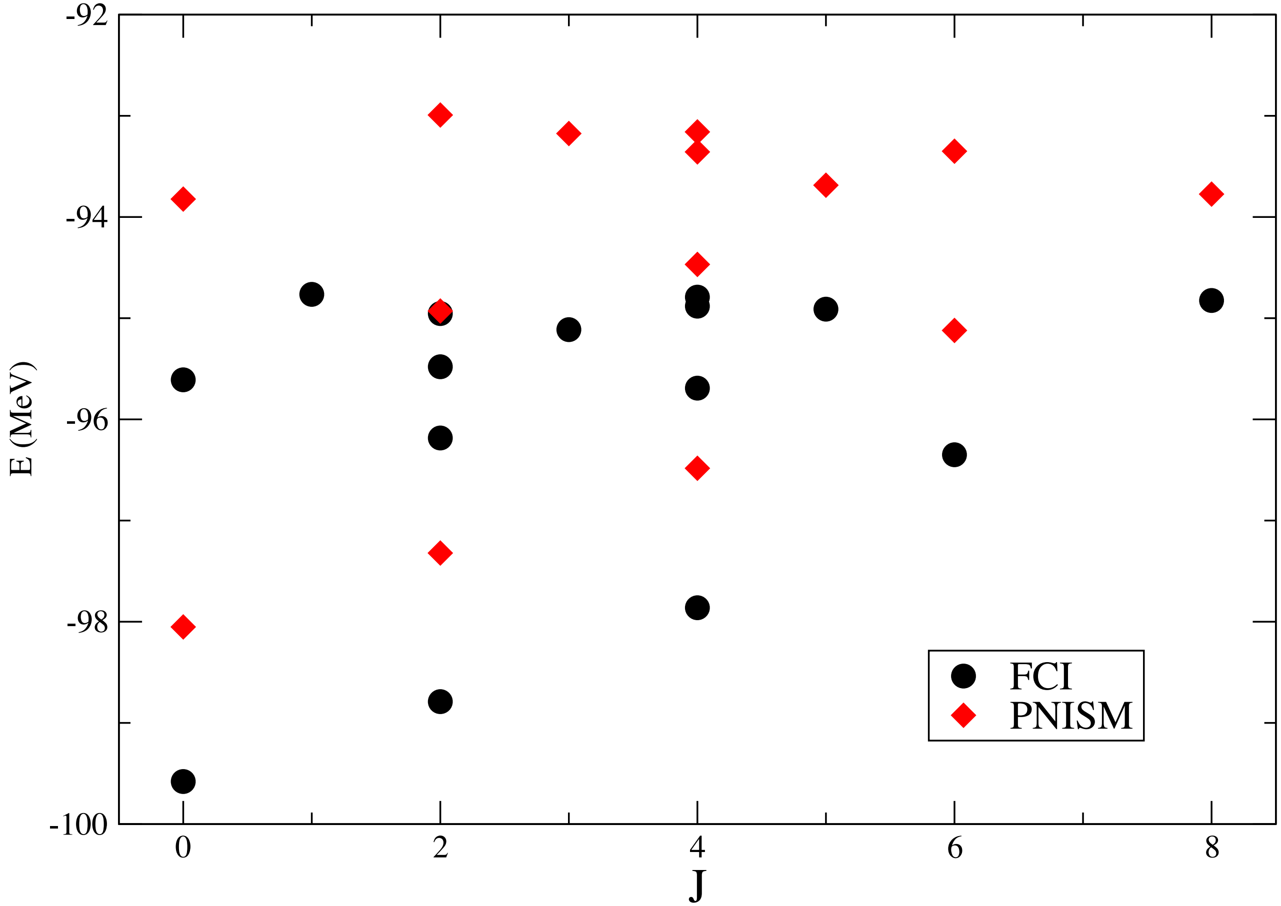


^{48}Cr, GX1A interaction



^{48}Cr

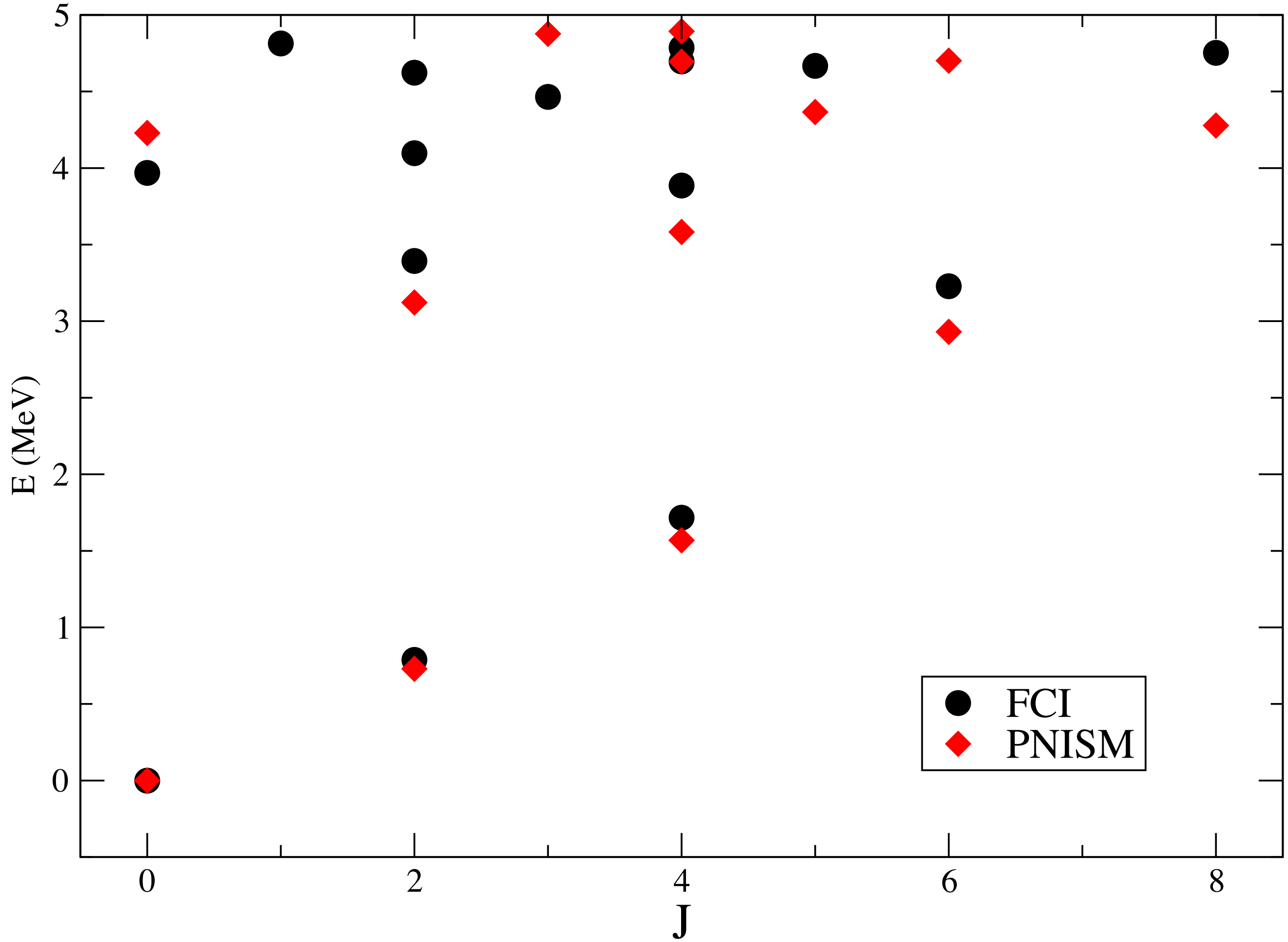
Absolute energies



40 proton levels + 40 neutron levels

^{48}Cr

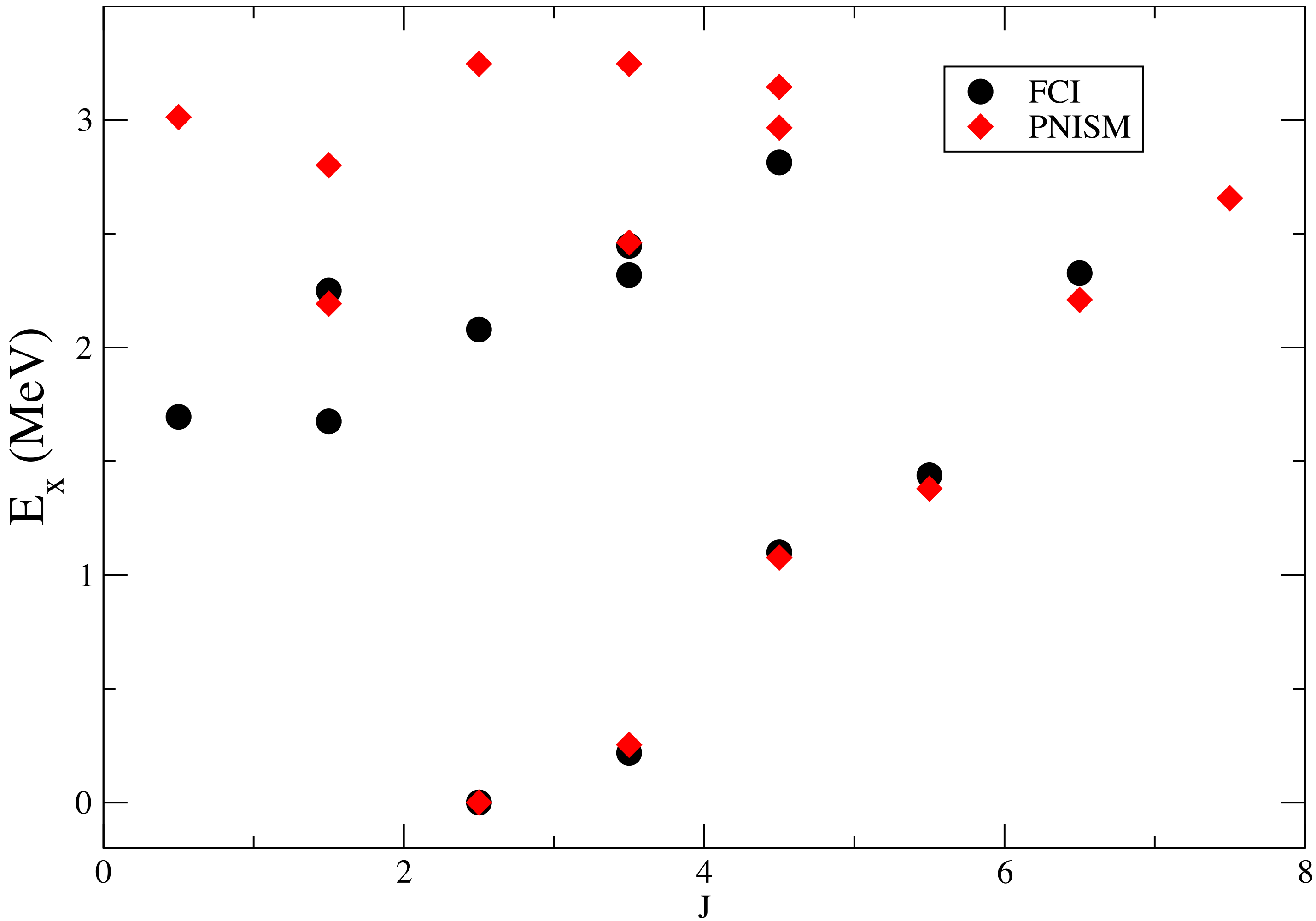
Excitation energies



40 proton levels + 40 neutron levels

^{49}Cr

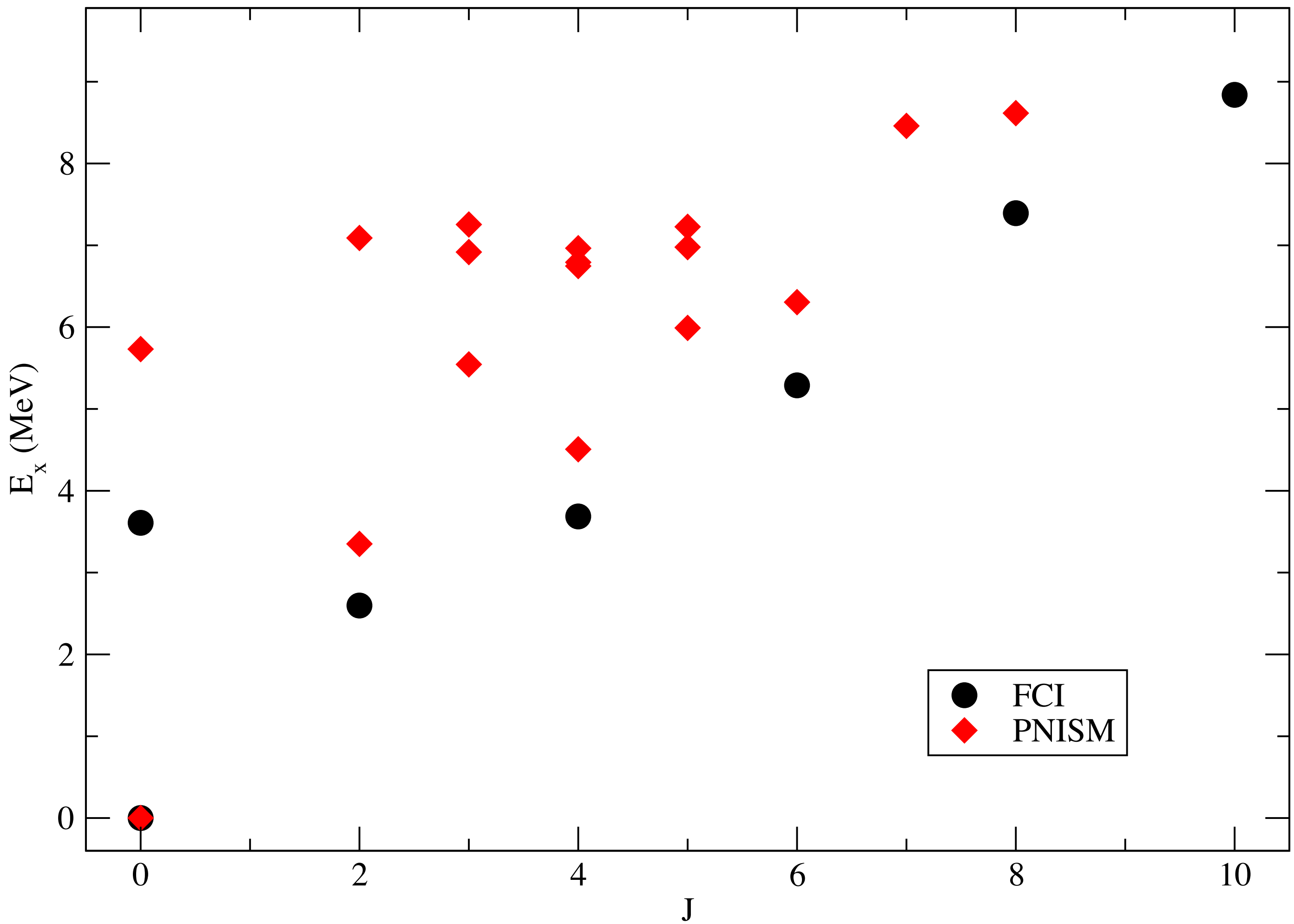
Excitation energies



40 proton levels + 40 neutron levels

^{56}Ni

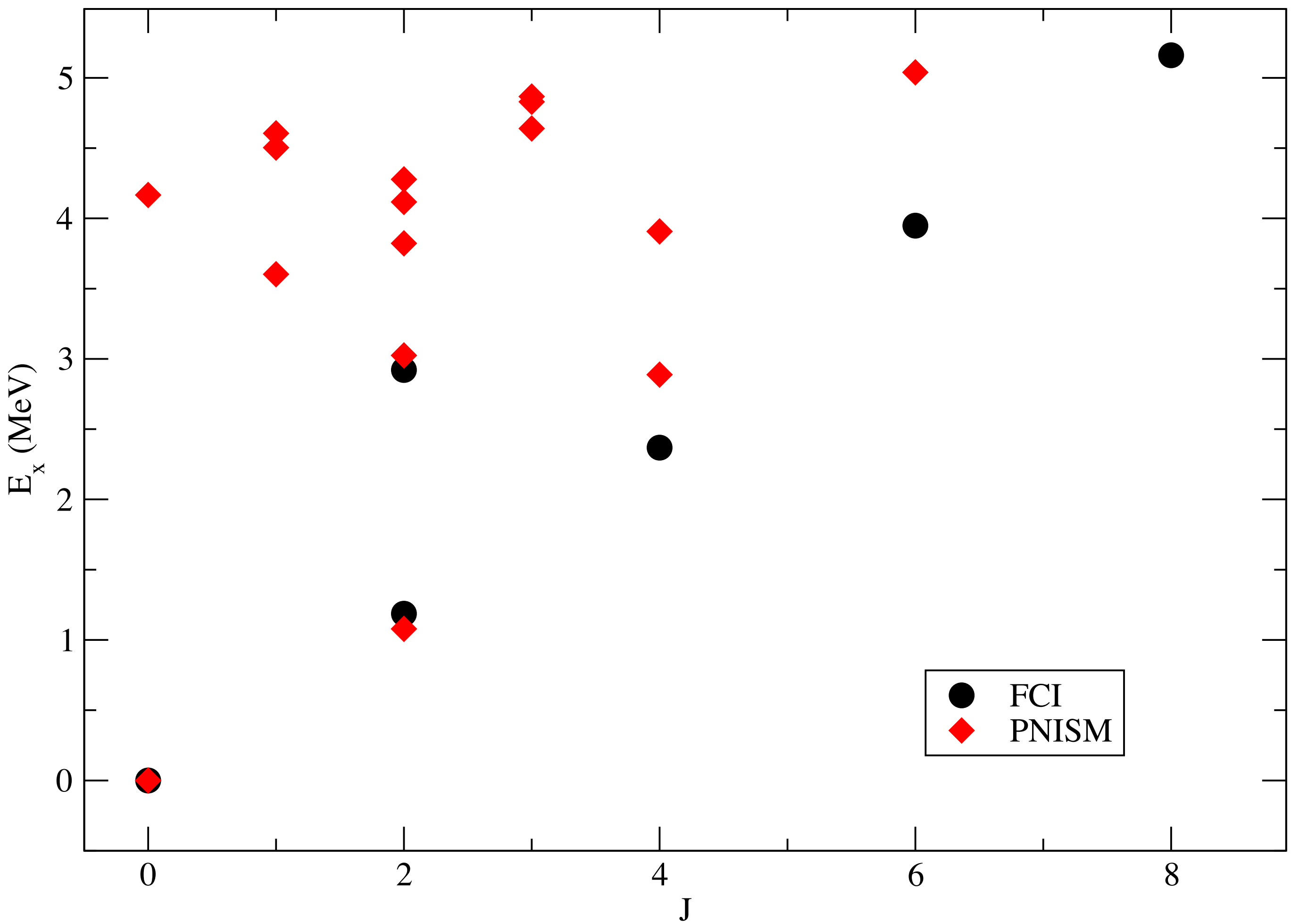
Excitation energies



40 proton levels + 40 neutron levels

^{60}Zn

Excitation energies



40 proton levels + 40 neutron levels

^{57}Fe
Excitation energies

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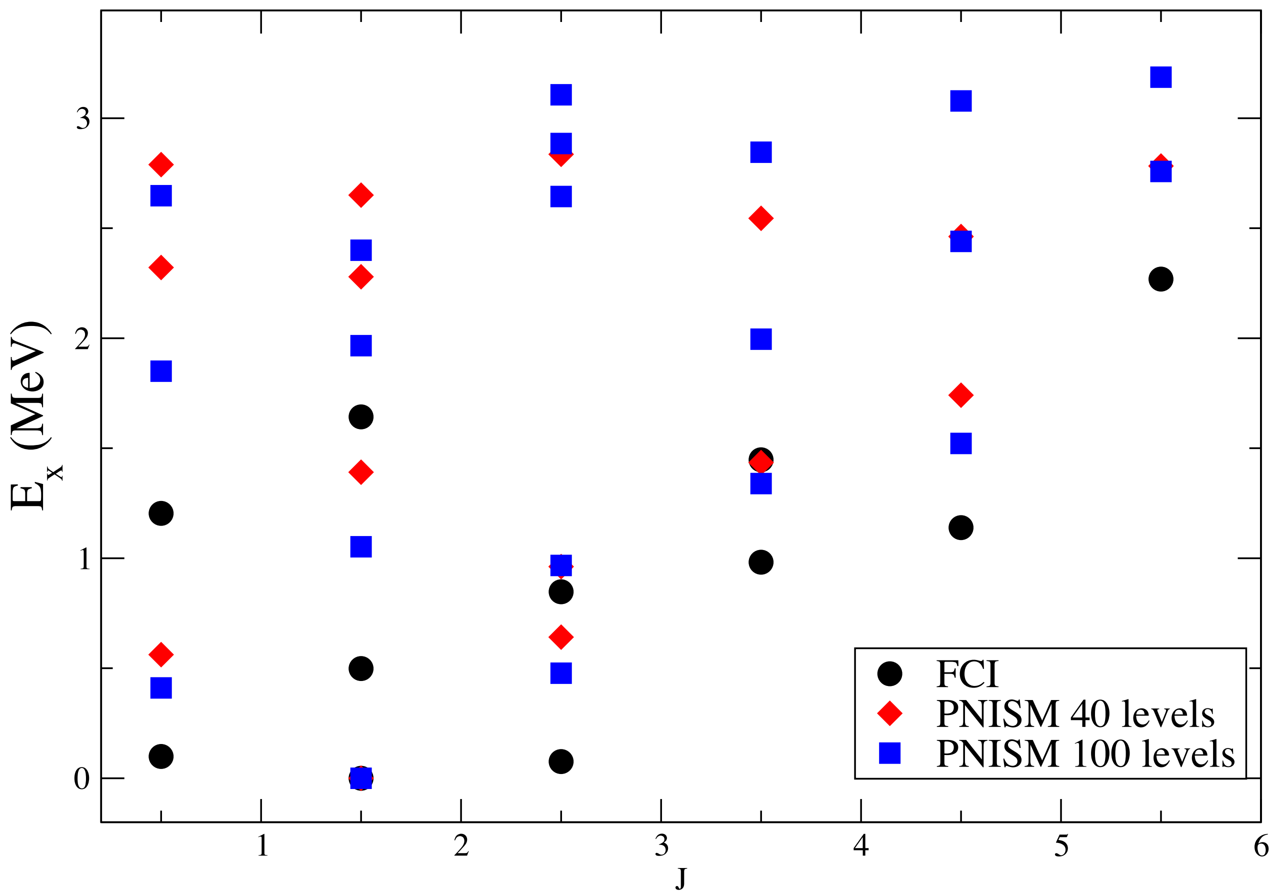

40 proton levels
+ 40 neutron
levels

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We have yet to do applications, only "proof of principle."

Sample application:
shells between 50 and 82 ($0g_{7/2}$ 2s1d $0h_{11/2}$)

^{129}Cs: M-scheme dim 50 billion (haven't tried!)

Proton dimension: 14,677
Neutron dimension: 646,430

We have yet to do applications, only "proof of principle."

Crazy-difficult isotope:
shells between 50 and 82 ($0g_{7/2}$ 2s1d $0h_{11/2}$)

^{132}Nd: M-scheme dim 85 TRILLION

Proton dimension =Neutron dimension= 3.7 million

Summary:

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- Shell model codes are restricted in size of problem; how to go further?

- BIGSTICK (and similar codes) use basis states which are simple outer products of proton, neutron states.

- Can we restrict ourselves to some subset of proton, neutron states?

- Use *entanglement entropy* to investigate.

* Looks promising, especially for $N \neq Z$

Next steps:

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- We have built a "weak *entanglement* code" PNISM
- Test transitions
- Make parallel/more efficient
- Investigate convergence
- Apply to currently intractable nuclides!

To detect dark matter,
one needs **nuclear cross-sections**.
For neutrino physics, **nuclear cross-sections**.
For neutrinoless ββ decay, **need nuclear matrix element**
For parity/time-reversal violation (e.g. EDM),
need nuclear matrix element....

EXTRA SLIDES

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Example of entanglement entropy: good angular momentum

Consider 2 spin-1/2 particles:

$$\left|\uparrow\uparrow\right\rangle, \left|\uparrow\downarrow\right\rangle, \left|\downarrow\uparrow\right\rangle, \left|\downarrow\downarrow\right\rangle$$

Example of entanglement entropy: good angular momentum

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Consider 2 spin-1/2 particles:

$$\left|\uparrow\uparrow\right\rangle, \left|\uparrow\downarrow\right\rangle, \left|\downarrow\uparrow\right\rangle, \left|\downarrow\downarrow\right\rangle$$

Consider total J=0 state: $\left|J=0\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$

then

$$\mathbf{C} = \begin{pmatrix} 0 & +\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$$

and

$$\rho_{\mu\mu'} = \sum_{\nu} c_{\mu\nu} c_{\mu'\nu}$$

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Example of entanglement entropy: good angular momentum

Consider total J=0 state: $\left| J=0 \right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle \right)$

then $\mathbf{c} = \begin{pmatrix} 0 & +\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$ and $\rho_{\mu\mu'} = \sum_{\nu} c_{\mu\nu} c_{\mu'\nu}$

or $\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$

Note trace ρ = 1.

Example of entanglement entropy: good angular momentum

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Consider total J=0 state: $\left|J=0\right\rangle = \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle - \left|\downarrow\uparrow\right\rangle\right)$

then $\mathbf{c} = \begin{pmatrix} 0 & +\frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & 0 \end{pmatrix}$ and $\rho_{\mu\mu'} = \sum_{\nu} c_{\mu\nu} c_{\mu'\nu}$

or $\rho = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$

Then entropy S = ln 2, which is the maximum.

Note trace ρ = 1.

Example of entanglement entropy: good angular momentum

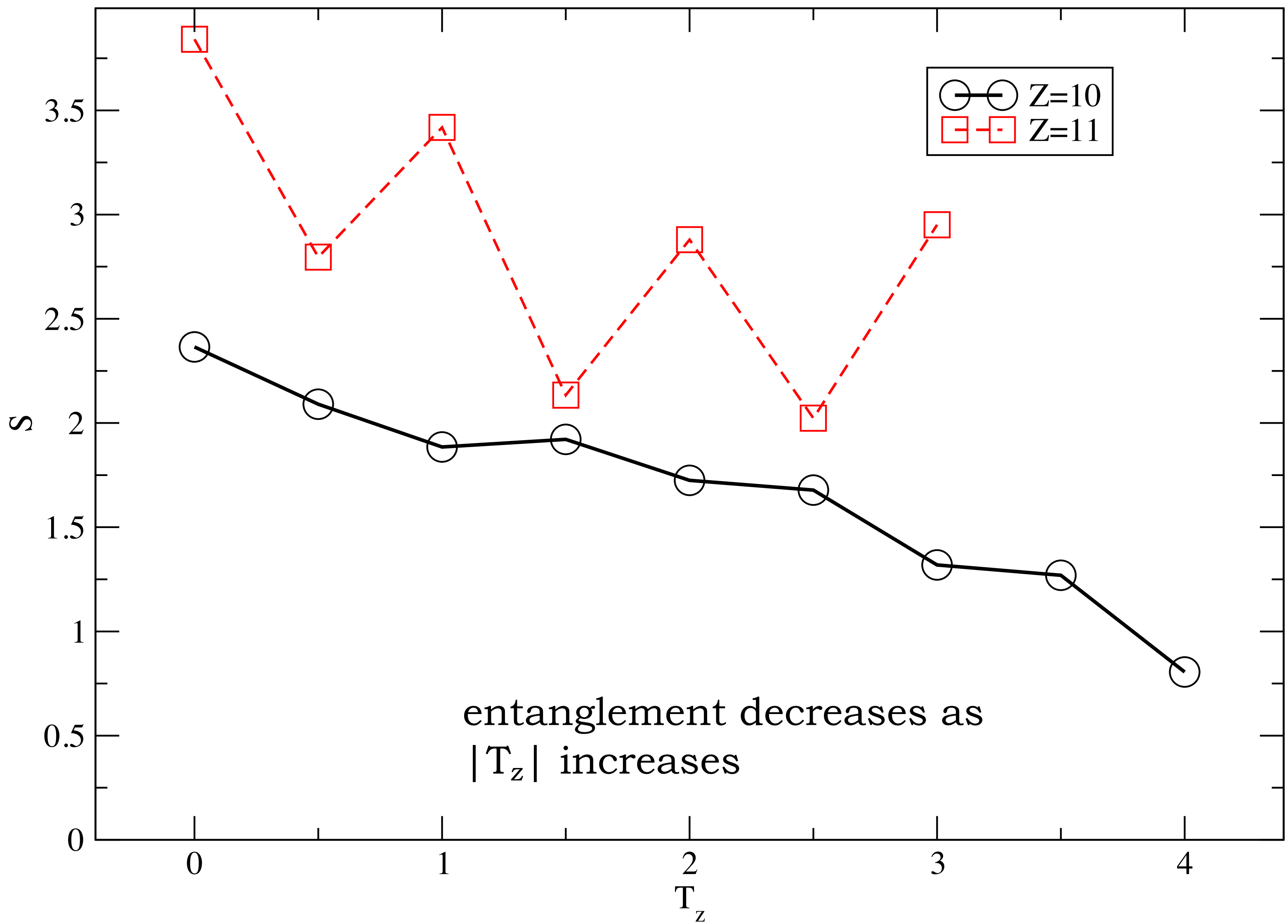
Conversely, $$\left|J=1,M=1\right\rangle = \left|\uparrow\uparrow\right\rangle$$

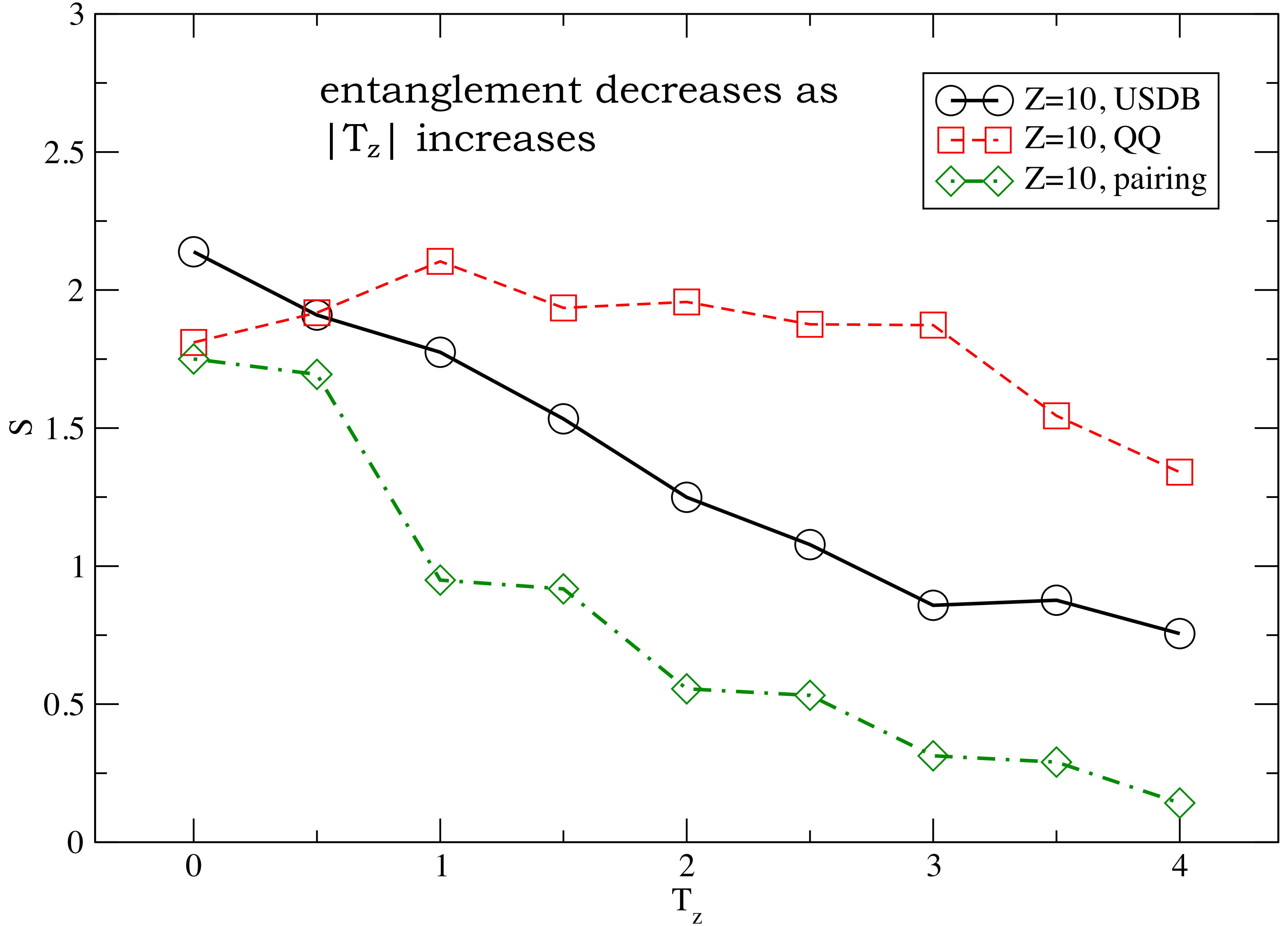
has $$\mathbf{C} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

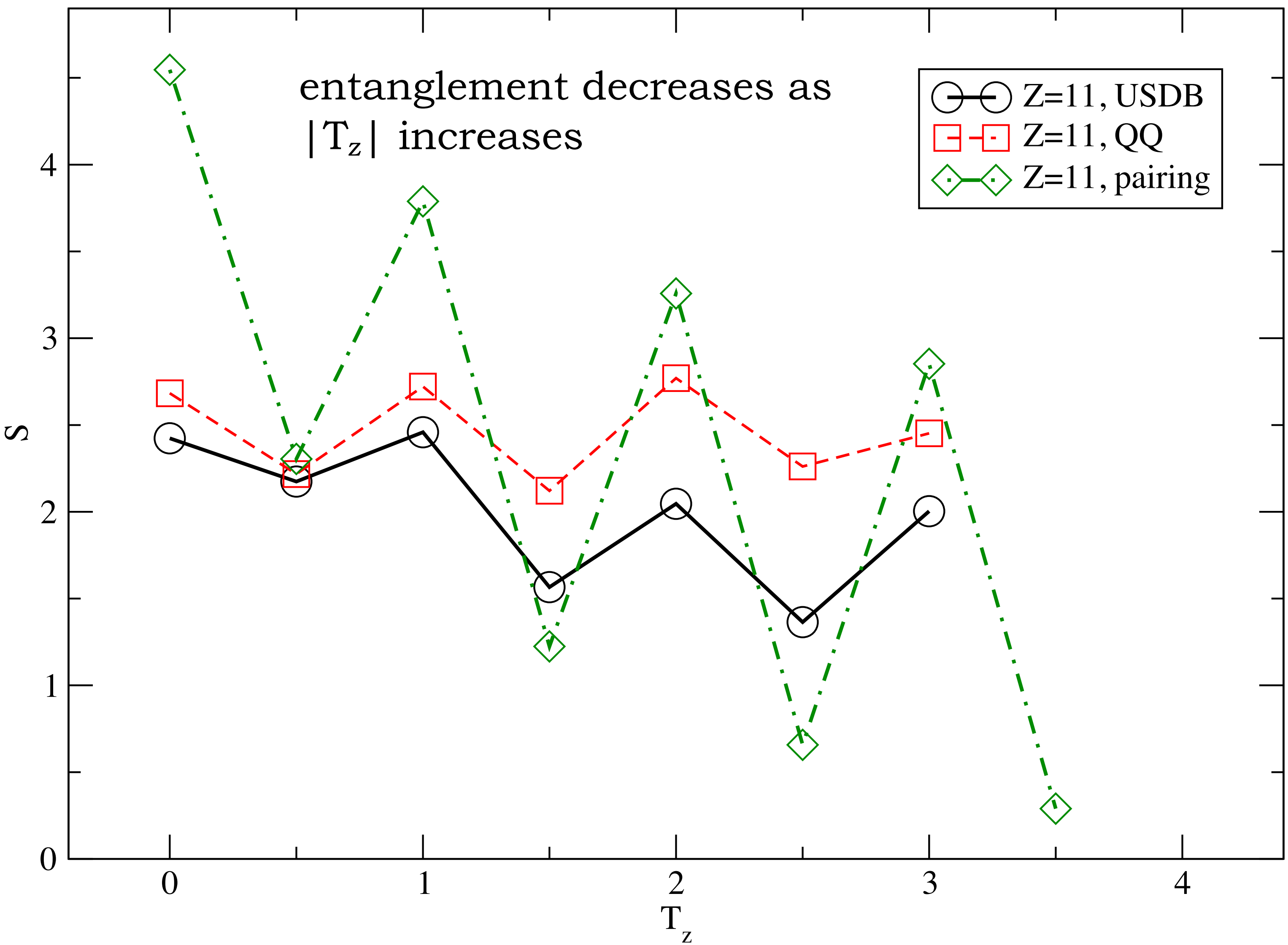
and $$\rho = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$ Then entropy $S = 0$.

Note trace $\rho = 1$.

USDB "traceless" = s.p.e, monopoles removed




entanglement decreases as
|T$_z$| increases
Z=10, USDB
Z=10, QQ
Z=10, pairing
S
T$_z$
0
0.5
1
1.5
2
2.5
3
4


entanglement decreases as
$|T_z|$ increases
Z=11, USDB
Z=11, QQ
Z=11, pairing
S
T_z
0
1
2
3
4
0
1
2
3
4

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That is, we take low-lying solutions of H_{pp} and H_{nn} and then project full solutions onto them

Let's decompose the wavefunction into eigenstates of H_{pp} and H_{nn}

Solve $$\left(\mathbf{H}_{pp}+\mathbf{H}_{nn}+\mathbf{H}_{pn}\right)\left|\Psi_{full}\right\rangle = E\left|\Psi_{full}\right\rangle$$

then solve $$\mathbf{H}_{pp}\left|\Psi_{p}\right\rangle = E_{p}\left|\Psi_{p}\right\rangle \qquad \mathbf{H}_{nn}\left|\Psi_{n}\right\rangle = E_{n}\left|\Psi_{n}\right\rangle$$

Expand $$\left|\Psi_{full}\right\rangle = \sum_{p,n} c_{p,n}\left|\Psi_{p}\right\rangle \otimes \left|\Psi_{n}\right\rangle$$

and compute P(p) $$= \left|\left\langle \Psi_{p} \middle| \Psi_{full}\right\rangle\right|^2 = \sum_{n} C_{p,n}^2$$

Solv

then s

I can do this efficiently using the "Lanczos trick"

Expand

$$\ldots_{full}\rangle = \sum_{p,n} c_{p,n} \left|\Psi_p\right\rangle \otimes \left|\Psi_n\right\rangle$$

ıpute P(p) $= \left|\left\langle \Psi_p \middle| \Psi_{full} \right\rangle\right|^2 = \sum_n C_{p,n}^2$

Although BIGSTICK is an M-scheme code

$$\left|\Psi, M\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu, M_p\right\rangle \left|n_\nu, M_n = M - M_p\right\rangle$$

because **H** commutes with $\mathbf{J}^2$, the eigenstates have good J

$$\left|\Psi, JM\right\rangle = \sum_{\mu\nu} c_{\mu\nu} \left|p_\mu, M_p\right\rangle \left|n_\nu, M_n = M - M_p\right\rangle$$

This is true even if only protons or only neutrons

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Technical details (if time allows)

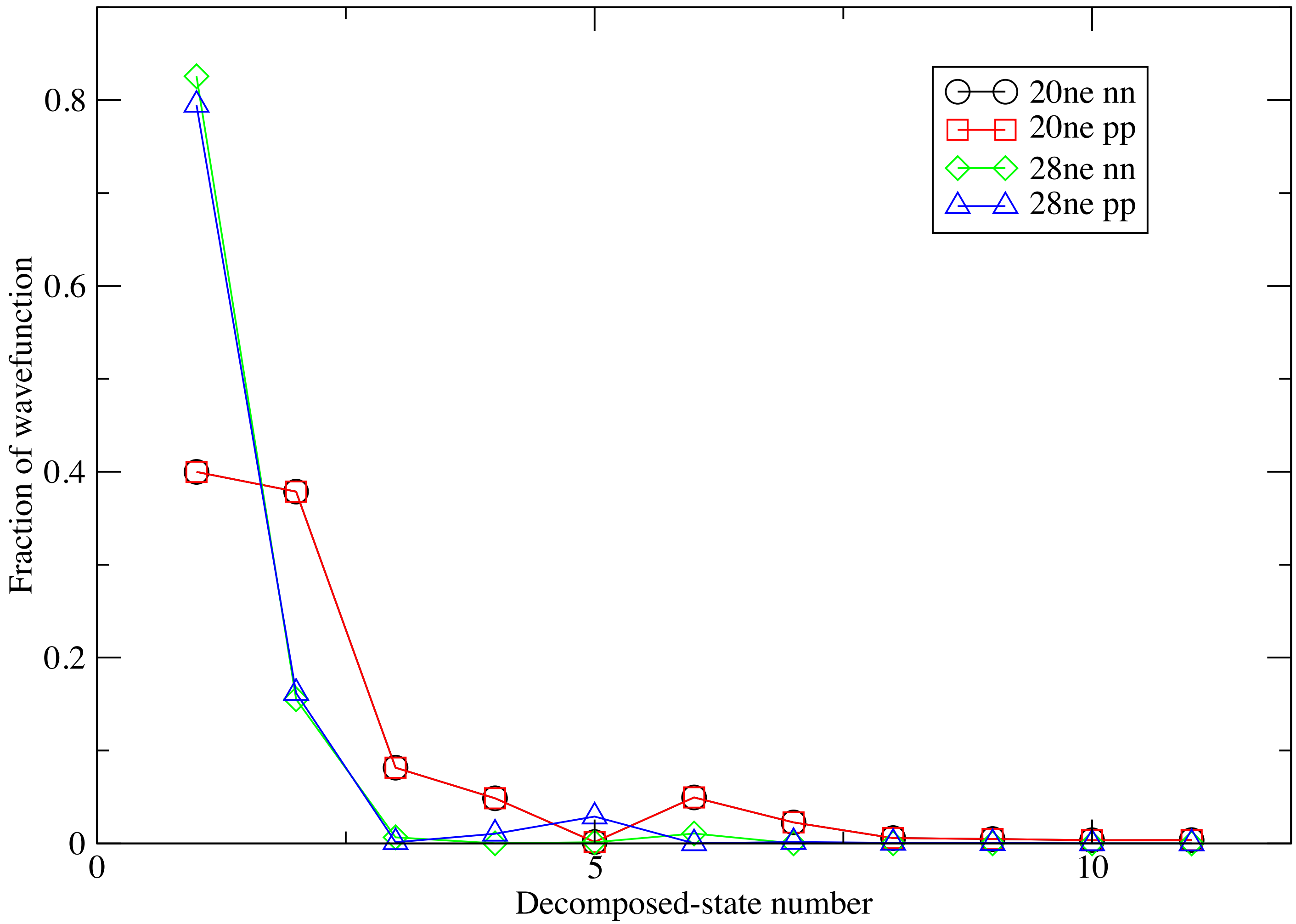
Let $\mathbf{H} = \mathbf{H}_{pp} + \mathbf{H}_{nn} + \mathbf{H}_{pn}$

BIGSTICK:
generate states $|a_p\rangle$, matrix elements $\langle a_p | \mathbf{H}_{pp} | a'_p \rangle$
and one body densities $\langle a_p | c^+_i c_j | a'_p \rangle$

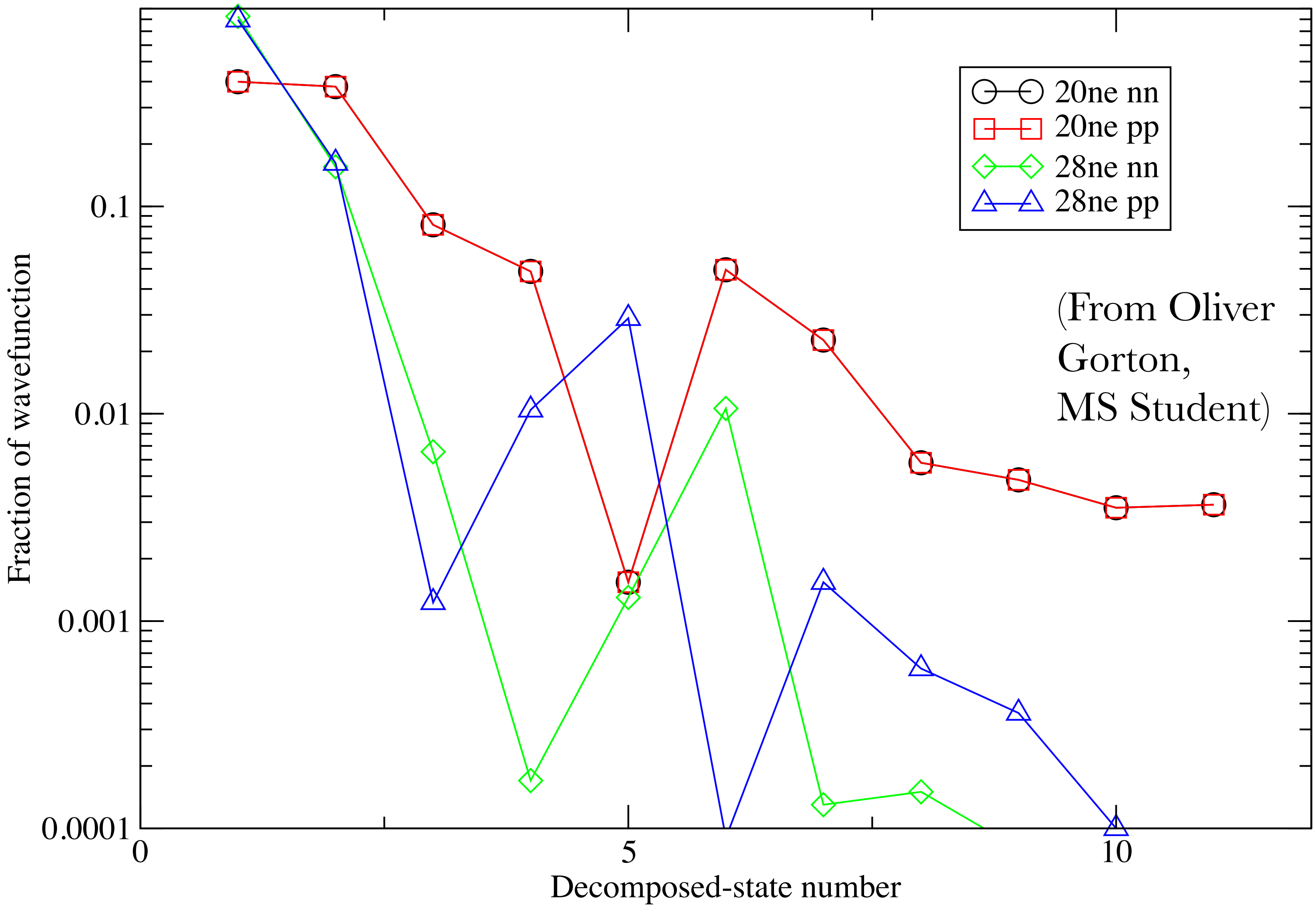
generate states $|b_n\rangle$, matrix elements $\langle b_n | \mathbf{H}_{nn} | b'_n \rangle$
and one body densities $\langle b_n | c^+_i c_j | b'_n \rangle$

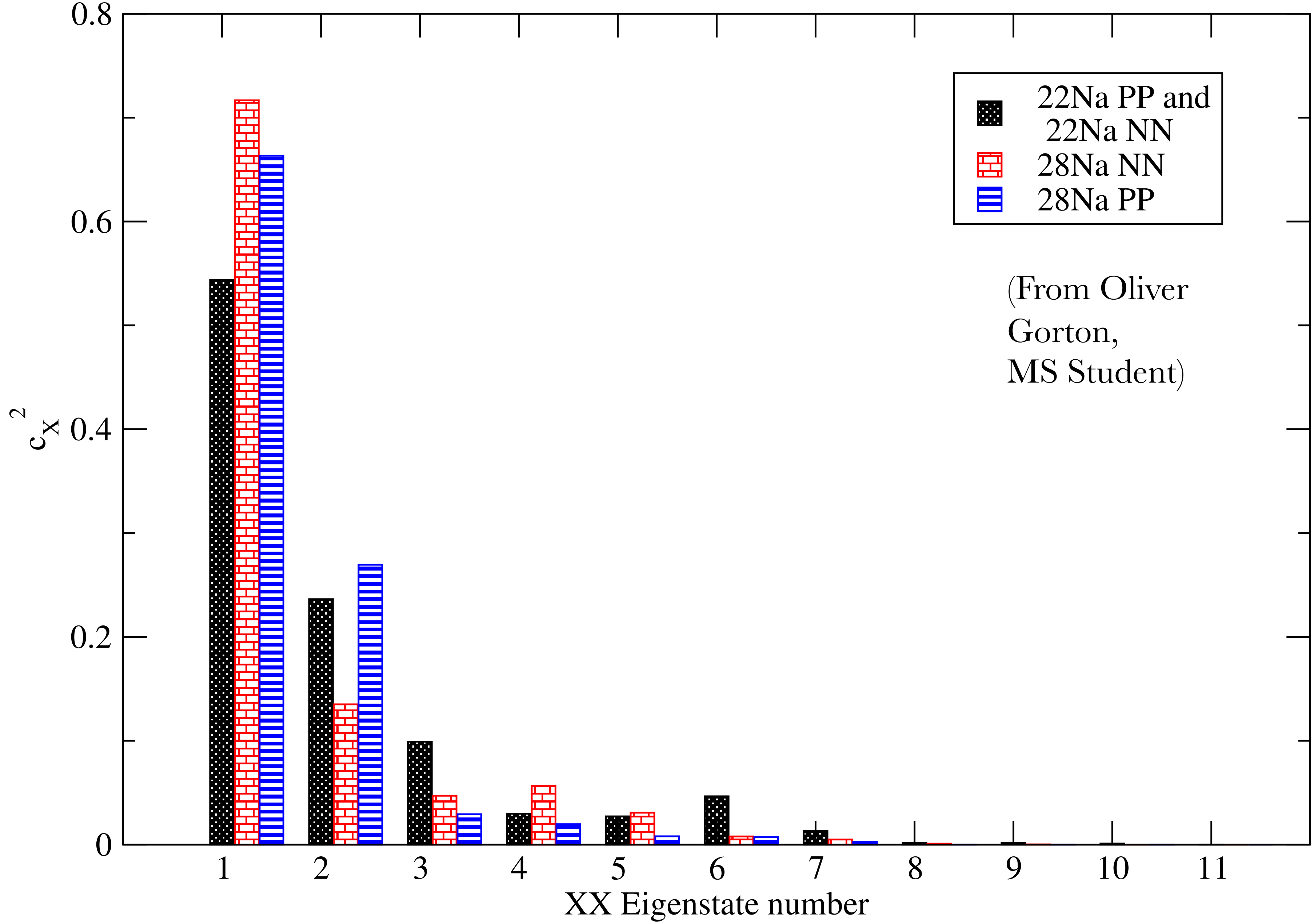
PNISM (proton-neutron interacting shell model)
read in the above and
generate matrix elements $\langle a_p , b_n | \mathbf{H}_{pn} | a'_p , b'_n \rangle$
using proton, neutron one-body densities

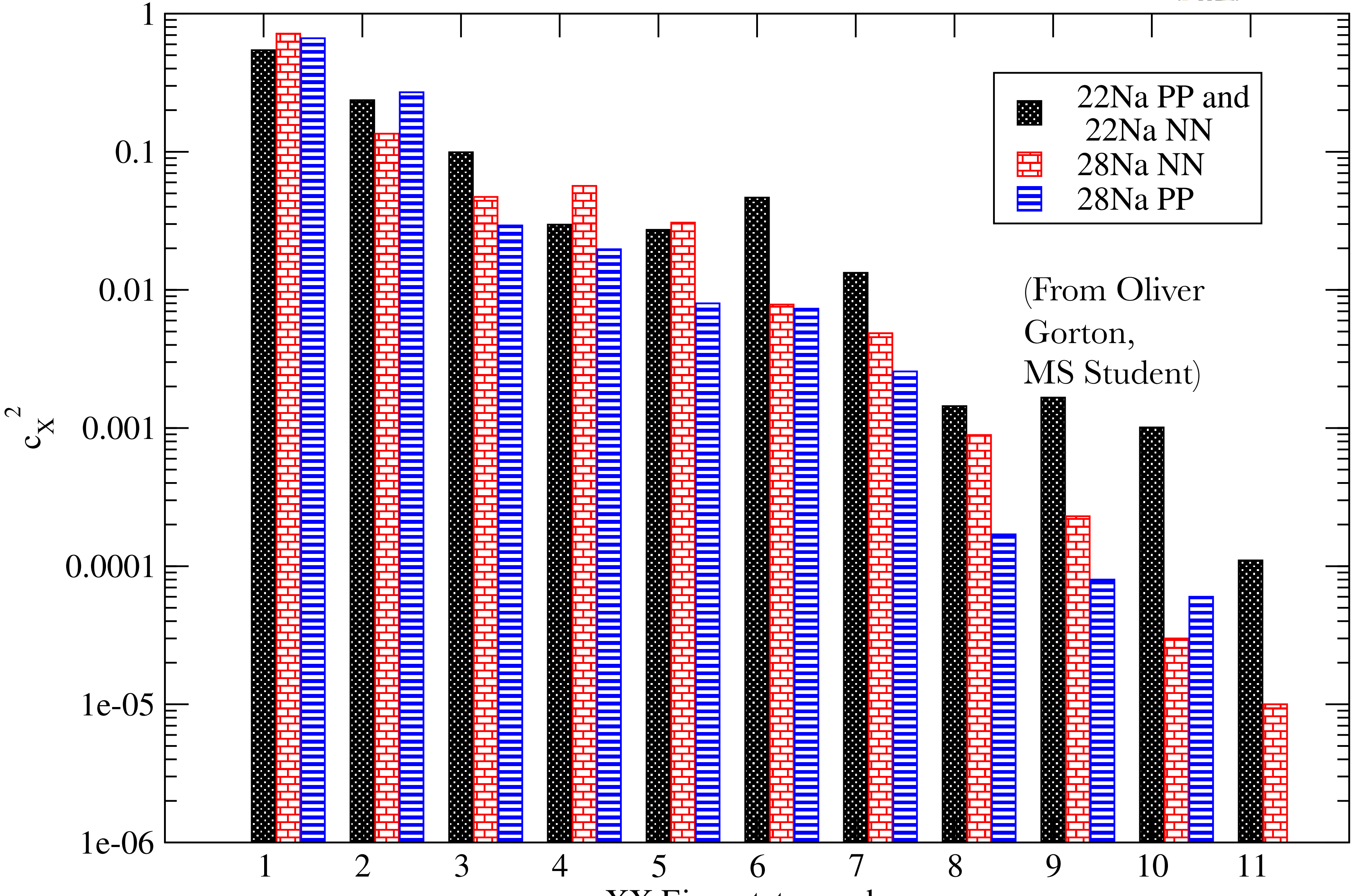
Diagonalize $\mathbf{H}_{pp} + \mathbf{H}_{nn} + \mathbf{H}_{pn}$ in truncated space.



20ne nn
20ne pp
28ne nn
28ne pp
Fraction of wavefunction
Decomposed-state number
0
0.2
0.4
0.6
0.8
0
5
10


20ne nn
20ne pp
28ne nn
28ne pp
(From Oliver Gorton, MS Student)
Fraction of wavefunction
0.1
0.01
0.001
0.0001
0
5
10
Decomposed-state number


0.8
0.6
0.4
0.2
0
c_X^2
1 2 3 4 5 6 7 8 9 10 11
XX Eigenstate number
22Na PP and 22Na NN
28Na NN
28Na PP
(From Oliver Gorton, MS Student)


22Na PP and
22Na NN
28Na NN
28Na PP
(From Oliver
Gorton,
MS Student)
c_X^2
1
0.1
0.01
0.001
0.0001
1e-05
1e-06
1 2 3 4 5 6 7 8 9 10 11
XX Eigenstate number