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# Entanglement entropy and proton-neutron interactions

Calvin W. Johnson

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ESNT workshop on PN Pairing + Quartets, Saclay, Sept 2019



Two related questions about the structure of atomic nuclei:

1) Is there a **simple** picture in which to *understand* nuclear properties?

2) Is there an **efficient** scheme in which to *model* nuclear structure for applications (e.g., dark matter cross-sections,  $0\nu\beta\beta$  matrix elements,  $\nu$ -A scattering, etc.)?



Two related questions about the structure of atomic nuclei:

1) Is there a **simple picture in which to understand** nuclear properties?

What do we mean by  
“simple”?

2) Is there an **easy way to model** nuclear structure for applications (e.g., cross-sections,  $0\nu\beta\beta$  matrix elements,  $\nu$ -A scattering, etc.)?





Ideally, "simple" means a few degrees of freedom describe many behaviors qualitatively / quantitatively

mic nuclei:

1) Is there a simple description of nuclear properties?

and nuclear

What do we mean by "simple"?

2) Is there an simple structure for a  $0\nu\beta\beta$  matrix element (e.g.,  $\nu$ -A scattering, etc.)?

el nuclear cross-sections,







## Some simple pictures:

- Single-particle/ (deformed) mean-field;
- Single-quasiparticle (HFB);
- pair condensates (both like particles, and p-n);
- quartets;
- Group theoretical frameworks ( “simple” = dominated by few irreps);
- ....





Simplicity is defined relative to a “complete” picture, which here is *configuration-interaction*

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

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

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

The basis states here are  
shell-model Slater determinants



Simplified shell model approximations

The interacting shell model is useful here because it is flexible and is a superset of many of these approximations

$|\Psi\rangle$

$\alpha$

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

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# The BIGSTICK shell-model code is public!

Download from:

[github.com/cwjsdsu/BigstickPublic](https://github.com/cwjsdsu/BigstickPublic)

Manual at [arXiv:1801.08432](https://arxiv.org/abs/1801.08432)

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

[fribtheoryalliance.org](http://fribtheoryalliance.org)



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:  $^{48}\text{Cr}$ , dim 2 million, ~10 minutes on laptop

$^{52}\text{Fe}$ , dim 110 million, a few hours on modest workstation

$^{56}\text{Ni}$ , dim 1 billion, 1 day on advanced workstation

$^{60}\text{Zn}$ , 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 ( $0g_{7/2}$   $2s_{1/2}$   $0h_{11/2}$ )

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

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

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

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



Can we come up with an  
alternate ("simpler")  
approach?





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

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





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

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



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

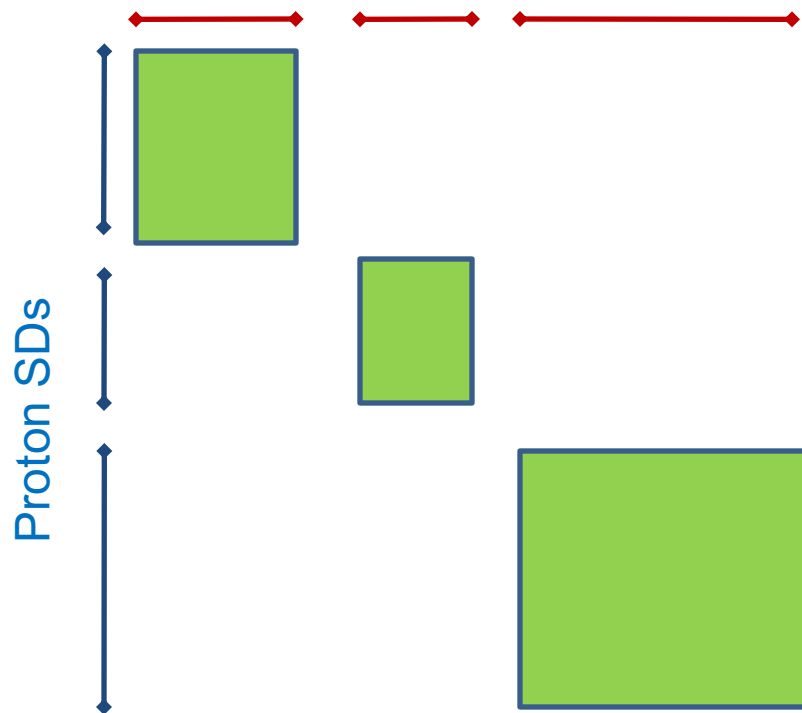
# FACTORIZATION



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

Neutron SDs



This leads to a block structure for construction of the basis



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

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



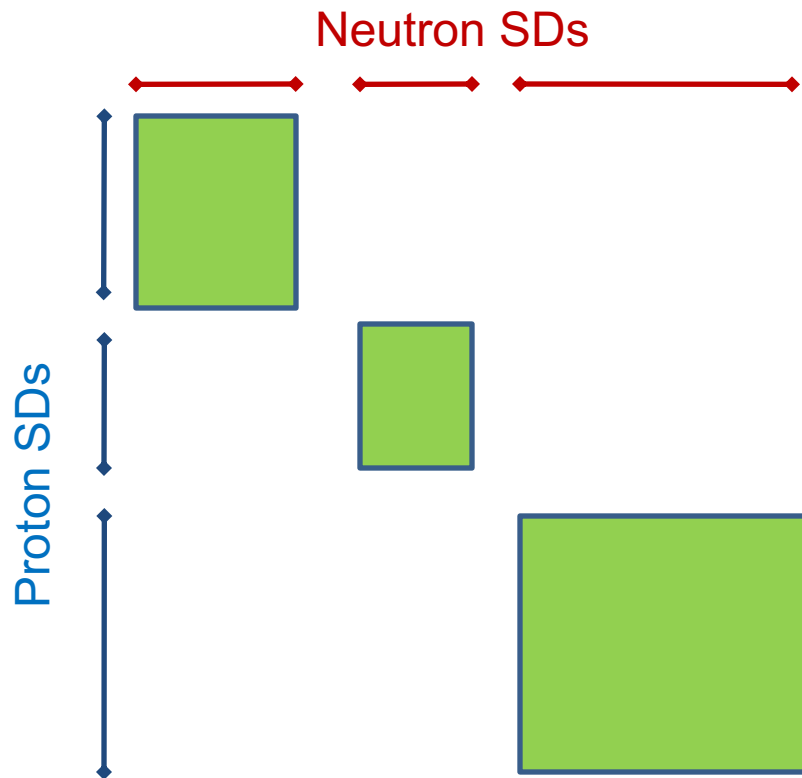
BIGSTICK exploits this  
for efficient representation  
of basis and Hamiltonian

# FACTORIZATION



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




Example N = Z nuclei

Nuclide	Basis dim	# pSDs (= #nSDs)
$^{20}\text{Ne}$	640	66
$^{24}\text{Mg}$	28,503	495
$^{28}\text{Si}$	93,710	924
$^{48}\text{Cr}$	1,963,461	4895
$^{52}\text{Fe}$	109,954,620	38,760
$^{56}\text{Ni}$	1,087,455,228	125,970



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

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



$$|01101000\dots\rangle |10010100\dots\rangle$$



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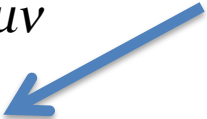
Alternate approach for medium/nuclei:  
Proton-neutron factorization

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

Can we truncate for just a few components?



Alternate approach for medium/nuclei:  
Proton-neutron factorization

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


$$(a_1|010110\dots\rangle + a_2|110010\dots\rangle + a_3|001011\dots\rangle + \dots)$$

No longer single “Slater determinants” but  
linear combinations...





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## Alternate approach for medium/nuclei: Proton-neutron factorization

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

Can we truncate for just a few components?

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



Alternate approach for medium/nuclei:  
Proton-neutron factorization

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

Can we truncate for just a few components?

(Alternate idea: truncated in each configuration/  
partition, e.g. Liao et al Phys. Rev. C 90, 024306)



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Example application:

shells between 50 and 82 ( $0g_{7/2}$   $2s_{1/2}$   $0h_{11/2}$ )

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

Proton dimension: 14,677

Neutron dimension: 646,430



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Example application:

$^{129}\text{Cs}$ : 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



So we want to ask:

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

These would not be single Slater determinants but linear combinations





So we want to ask:

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

In other words, is it “simple” in terms of coupling between proton and neutron building blocks





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My tool for investigation:  
The *entanglement entropy*

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

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

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



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My tool for investigation:  
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$$|\Psi\rangle = \sum_{\mu\nu} c_{\mu\nu} |p_{\mu}\rangle |n_{\nu}\rangle$$

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

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

$$S = -\sum_i \lambda_i \ln \lambda_i = -\text{tr} \rho \ln \rho$$





The *entanglement entropy*

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

$$S = -\sum_i \lambda_i \ln \lambda_i = -\text{tr} \rho \ln \rho$$

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



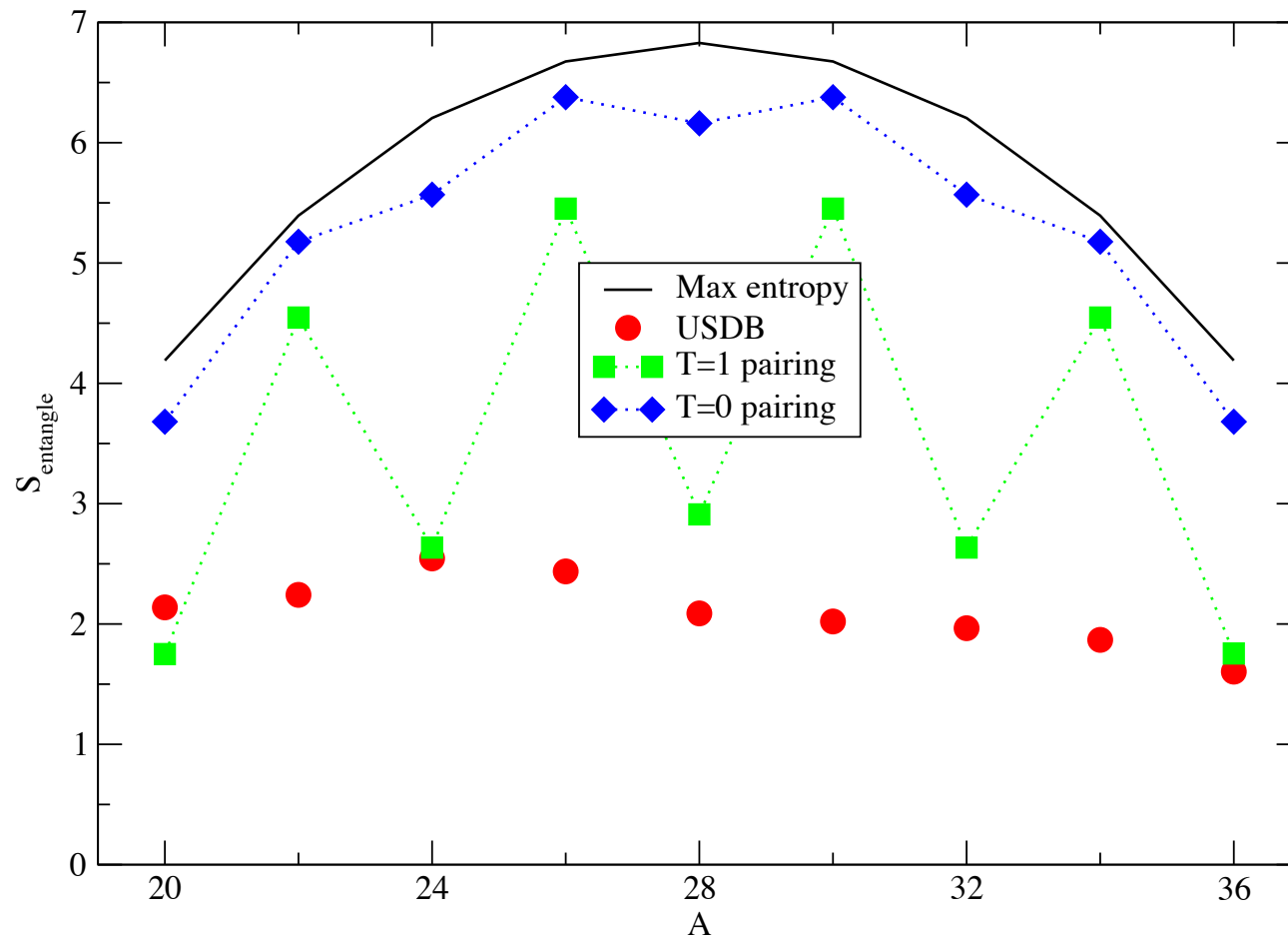
Now let's turn to nuclei, with

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

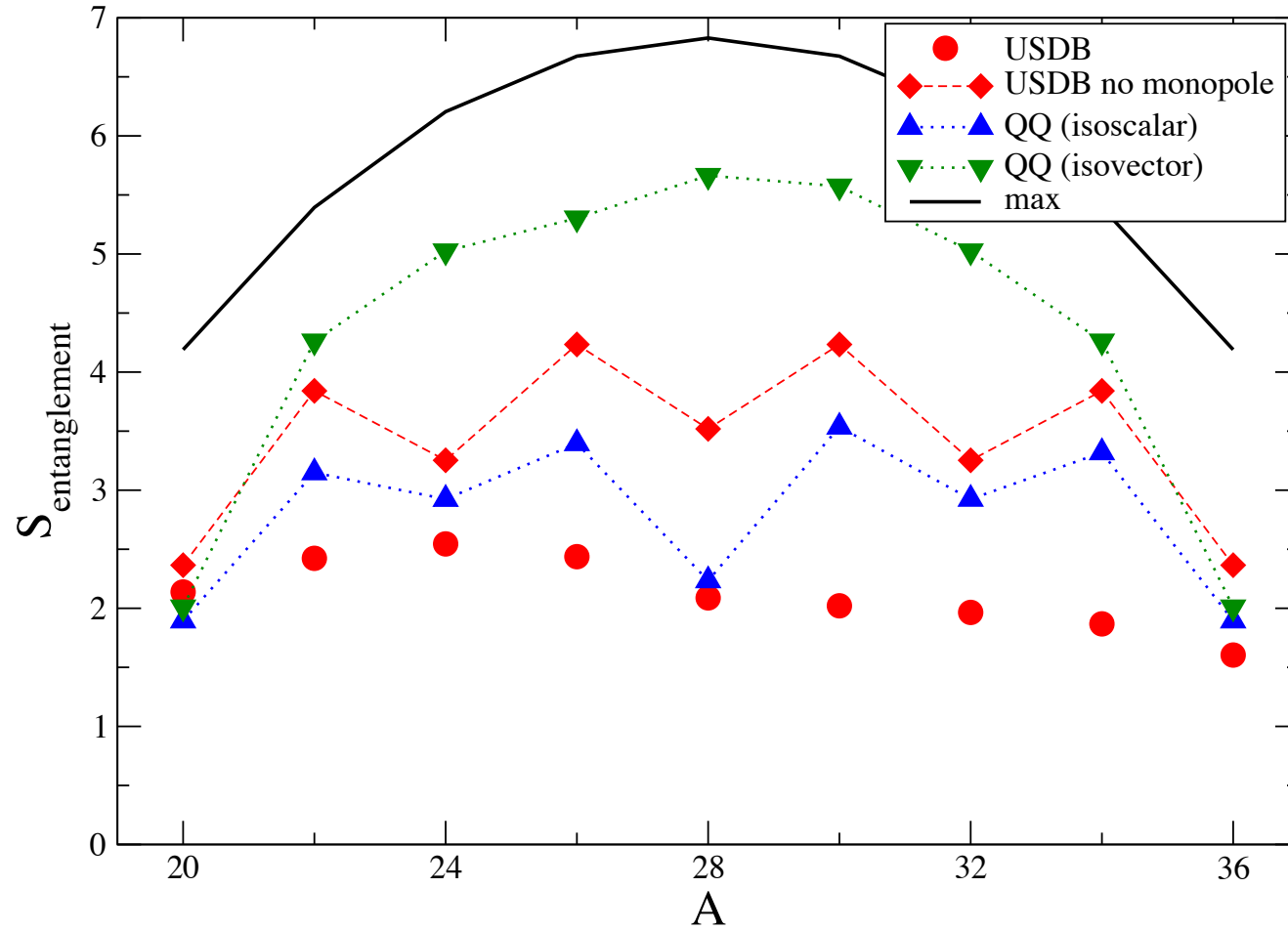




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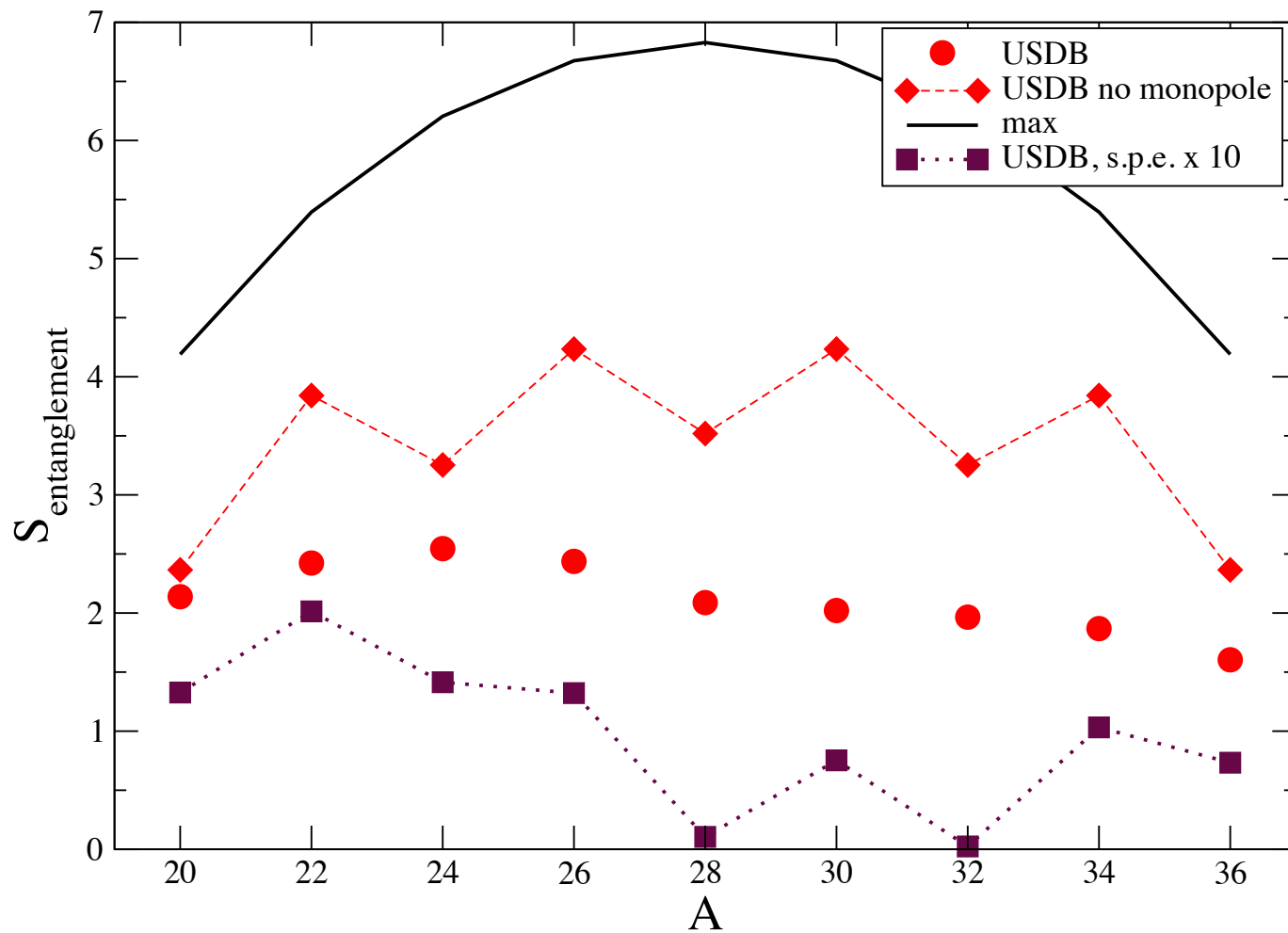
$Z=N$  nuclei  
in  $sd$  shell



Z=N nuclei  
in *sd* shell



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$Z=N$  nuclei  
in  $sd$  shell



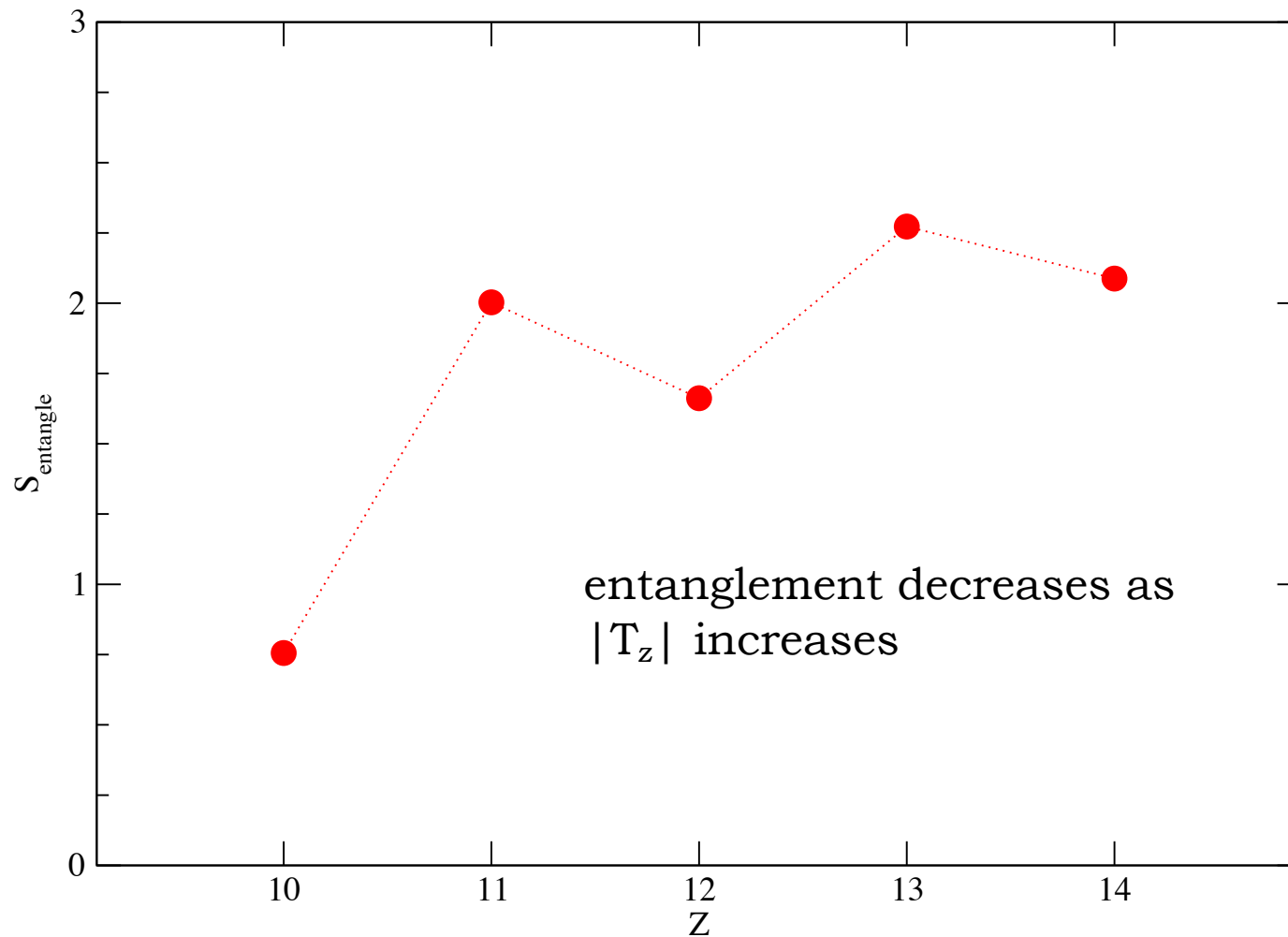
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Now let's follow  
as isospin increases





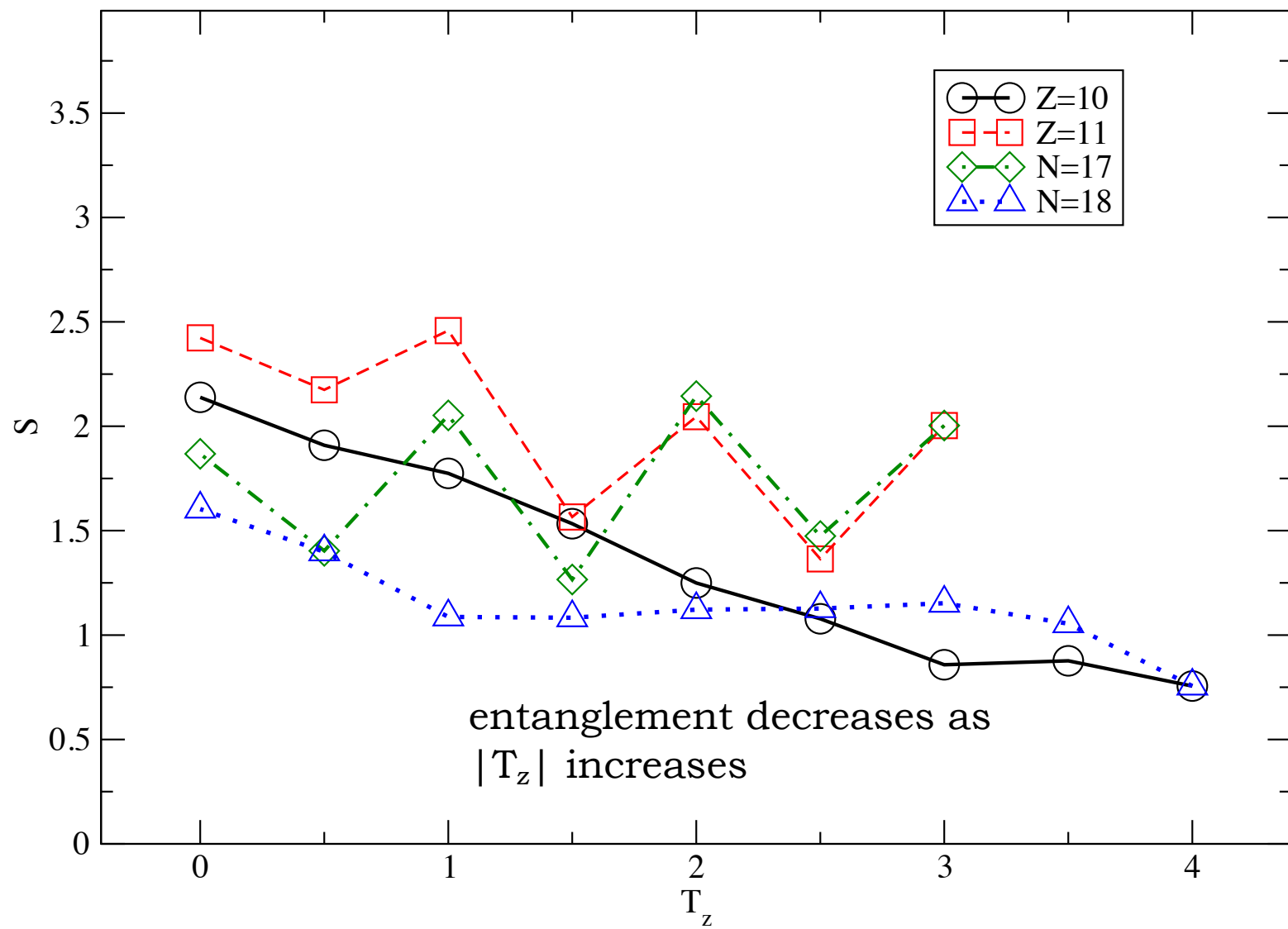
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$A=28$  nuclei  
in  $sd$  shell  
with USDB

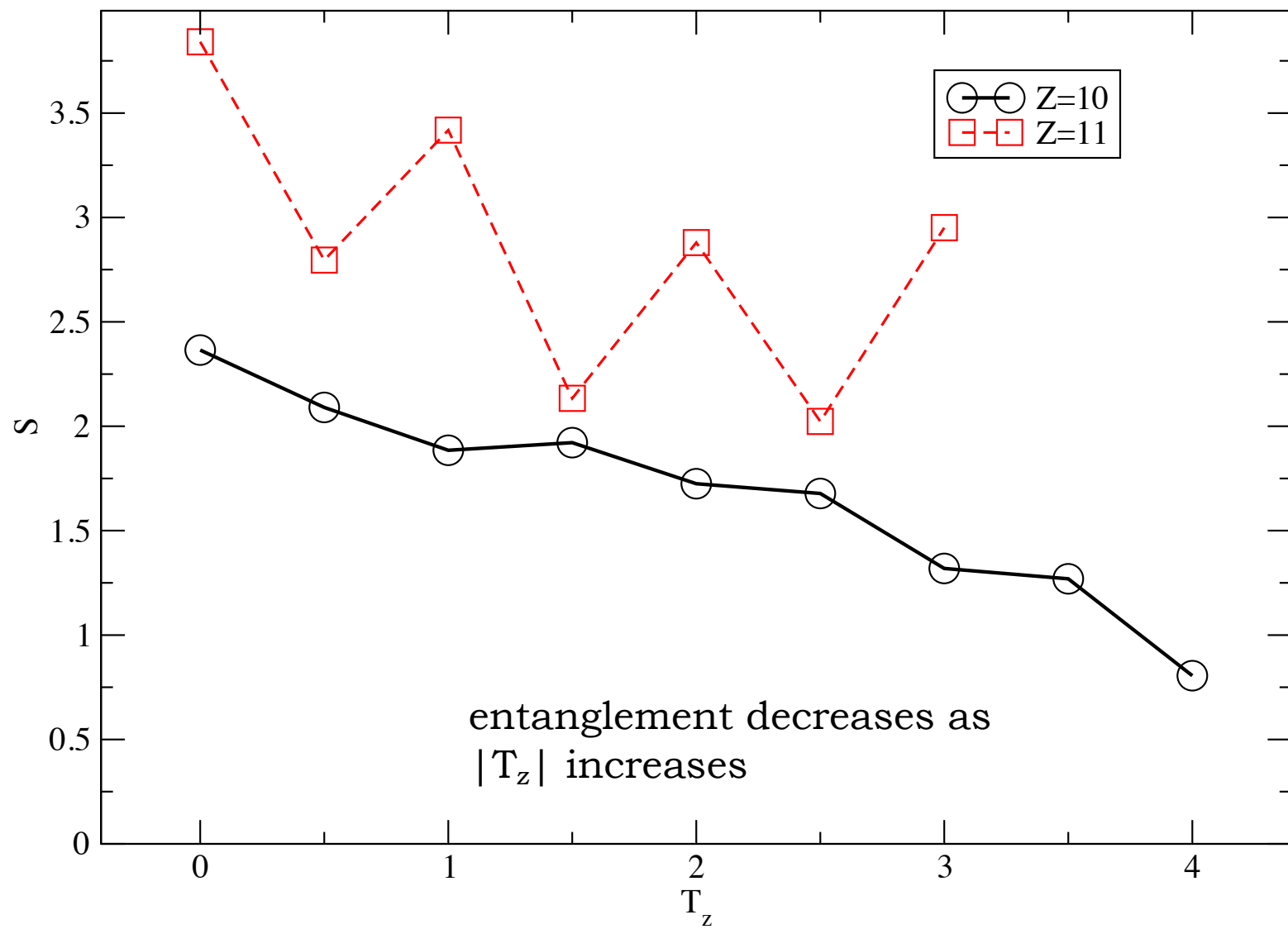
entanglement decreases as  
 $|T_z|$  increases

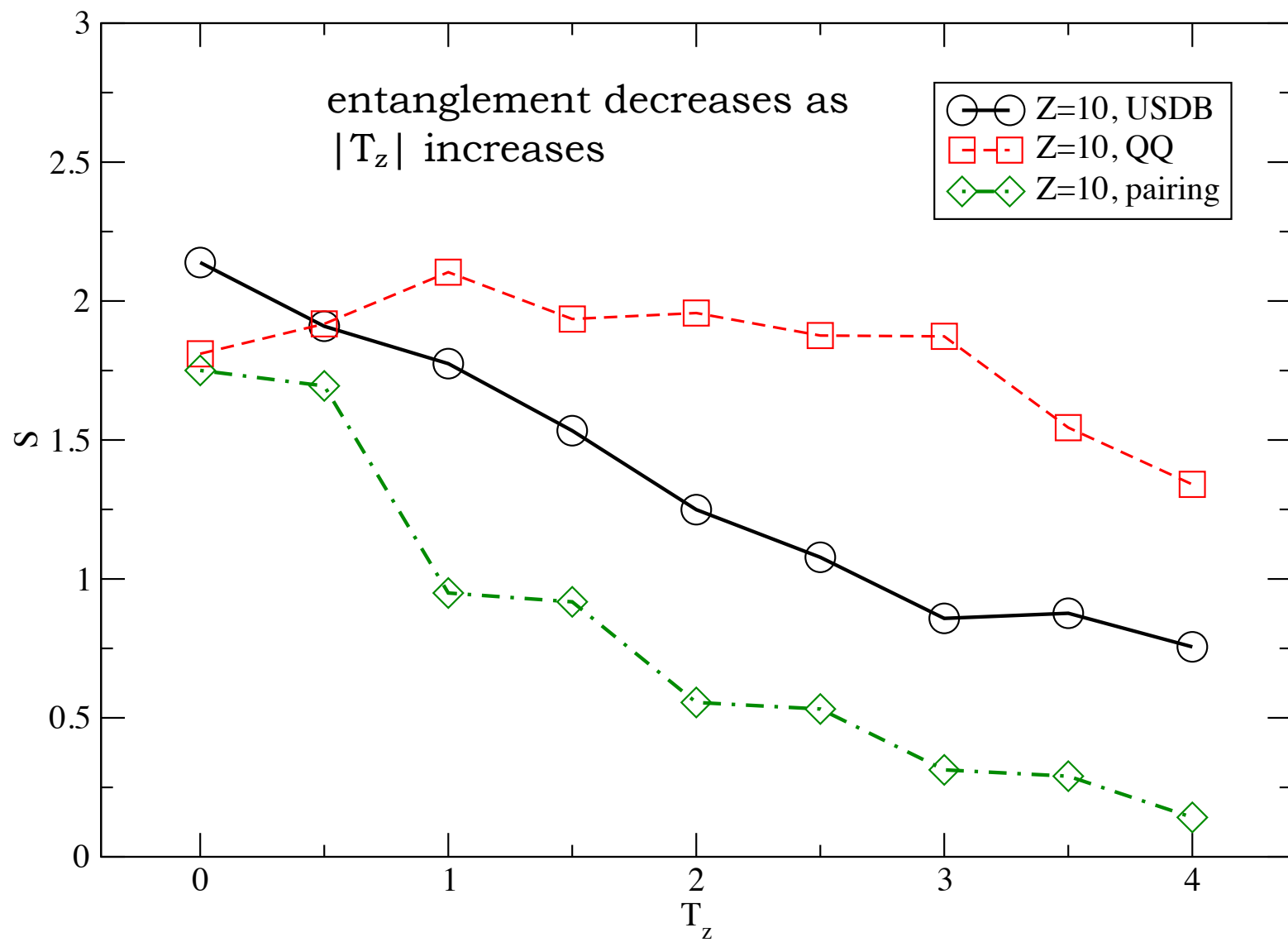
# USDB

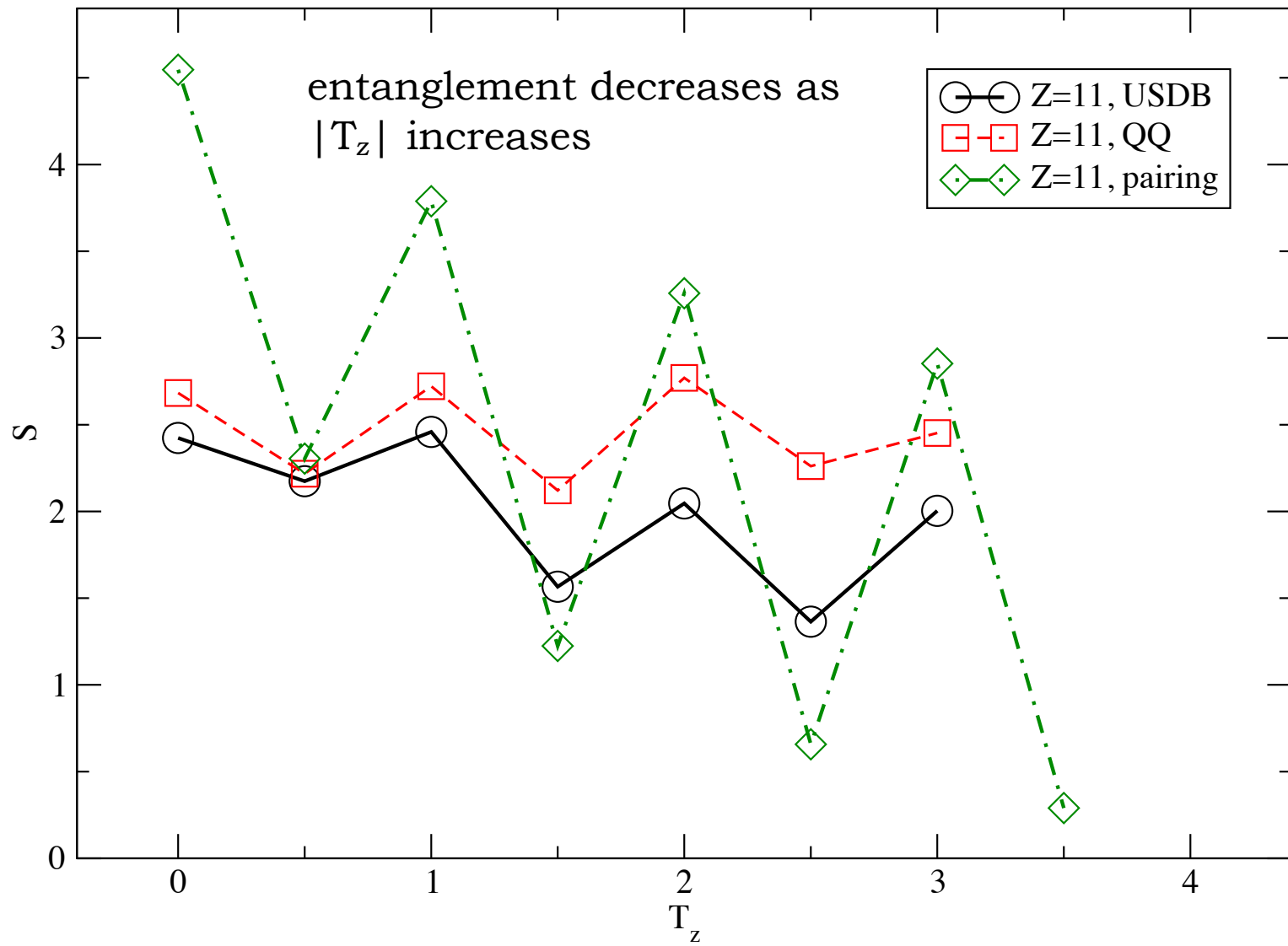




USDB "traceless" = s.p.e, monopoles removed





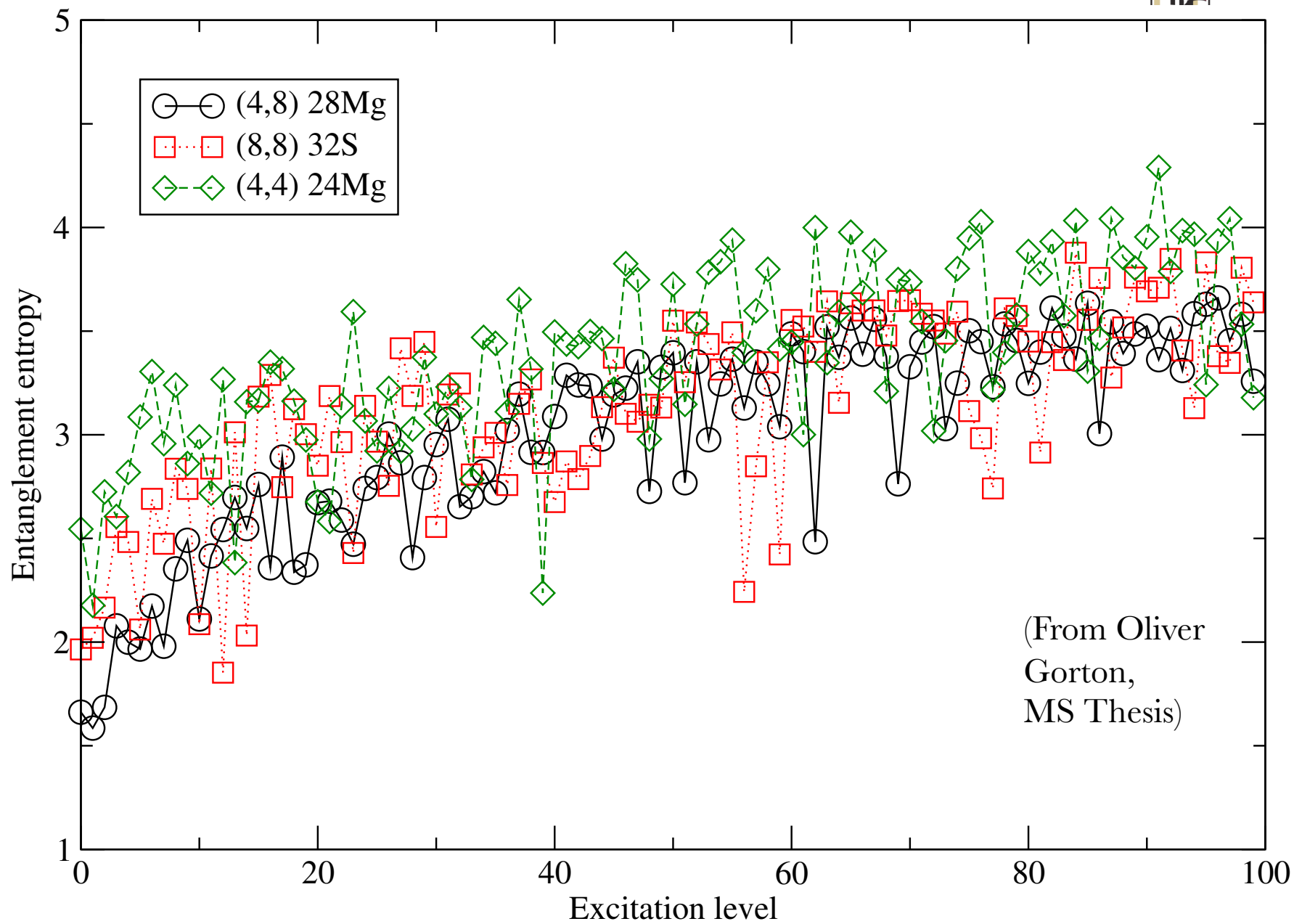




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What about as we increase  
in excitation energy?







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What about other partitions?

Like pairing, or quartets?





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It would be very interesting to look at the entanglement entropy of, say, single-particles, or pairs, or quartets.

These are independent tests of our ideas about mean-field pictures, or various ‘condensates’

However it’s not so easy if one wants to do it rigorously.



Let

$$|\Psi\rangle = \sum_{\alpha, i} c_{i, \alpha} \hat{a}_i^\dagger \hat{b}_\alpha^\dagger |0\rangle$$

How to find  $\rho_{ij} = \sum_{\alpha} c_{i, \alpha}^* c_{j, \alpha}$  ?

Especially if  $[\hat{a}_i, \hat{b}_\alpha^\dagger] \neq 0$  ?





Compute

$$\langle b_{\alpha} | \hat{a}_i | \Psi \rangle \quad \text{where} \quad | b_{\alpha} \rangle = \hat{b}_{\alpha}^{\dagger} | 0 \rangle$$

“spectroscopic factor”

but also need a density matrix

$$\langle b_{\alpha} | \hat{a}_i \hat{a}_j^{\dagger} | b_{\beta} \rangle$$



Then solve

$$\langle b_\alpha | \hat{a}_i | \Psi \rangle = \sum_{j,\beta} c_{j,\beta} \langle b_\alpha | \hat{a}_i \hat{a}_j^\dagger | b_\beta \rangle$$

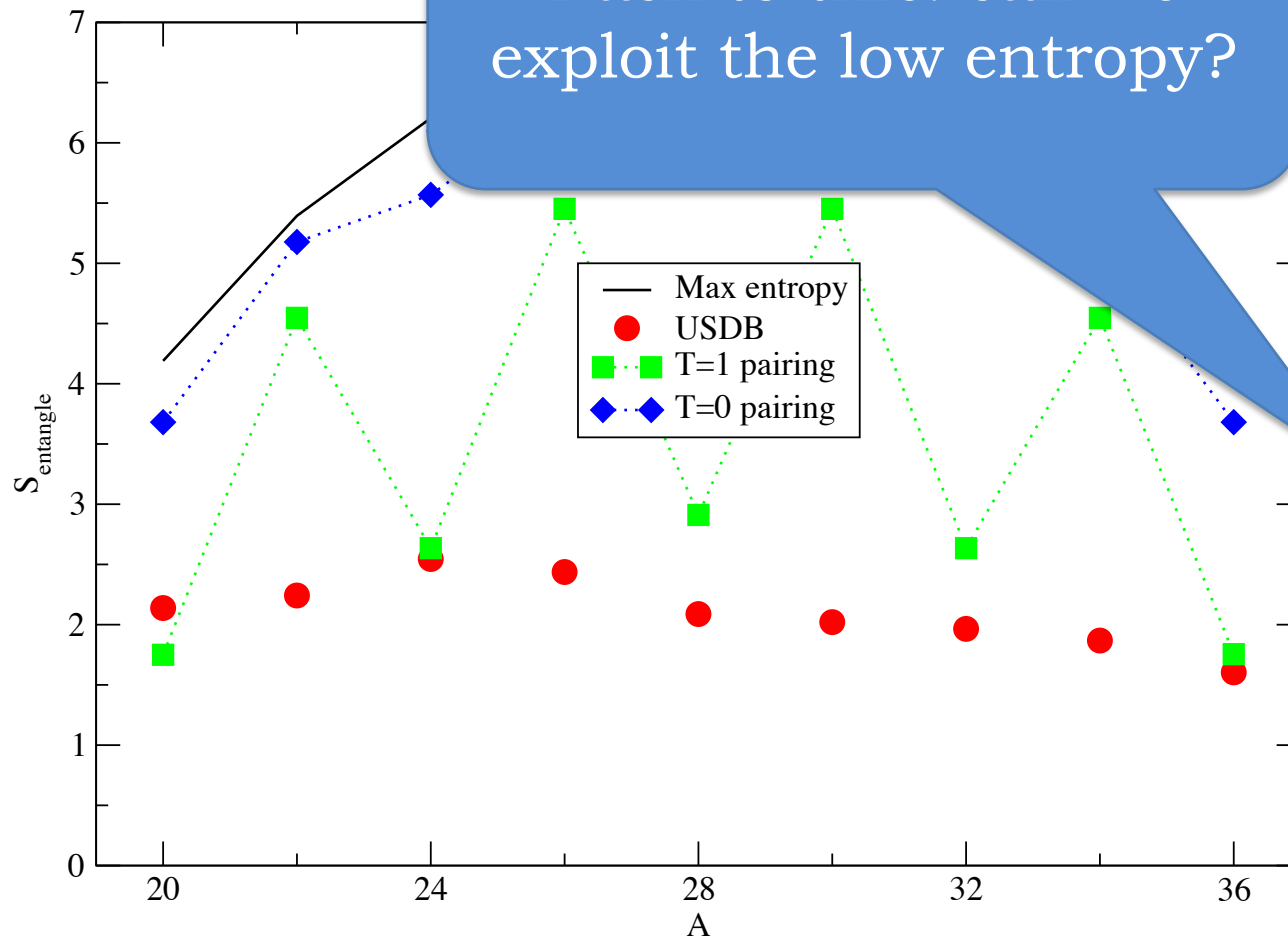
Highly nontrivial, but possible in modest-sized systems  
(not yet done)

→ could lead to “how simple” a wave function looks like  
in terms of “pairing” or “quartet” bases



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Back to this: can we  
exploit the low entropy?

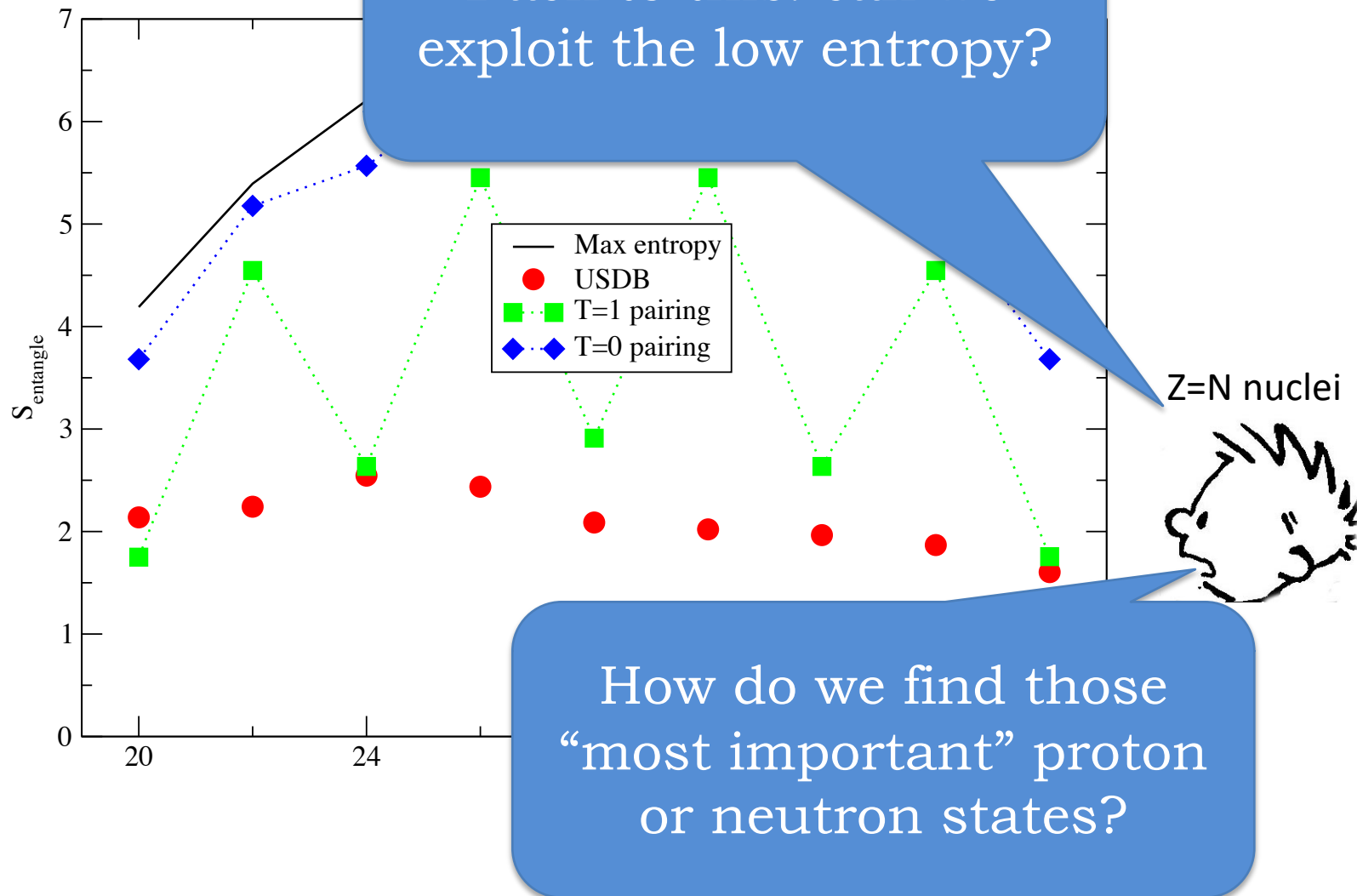


Z=N nuclei



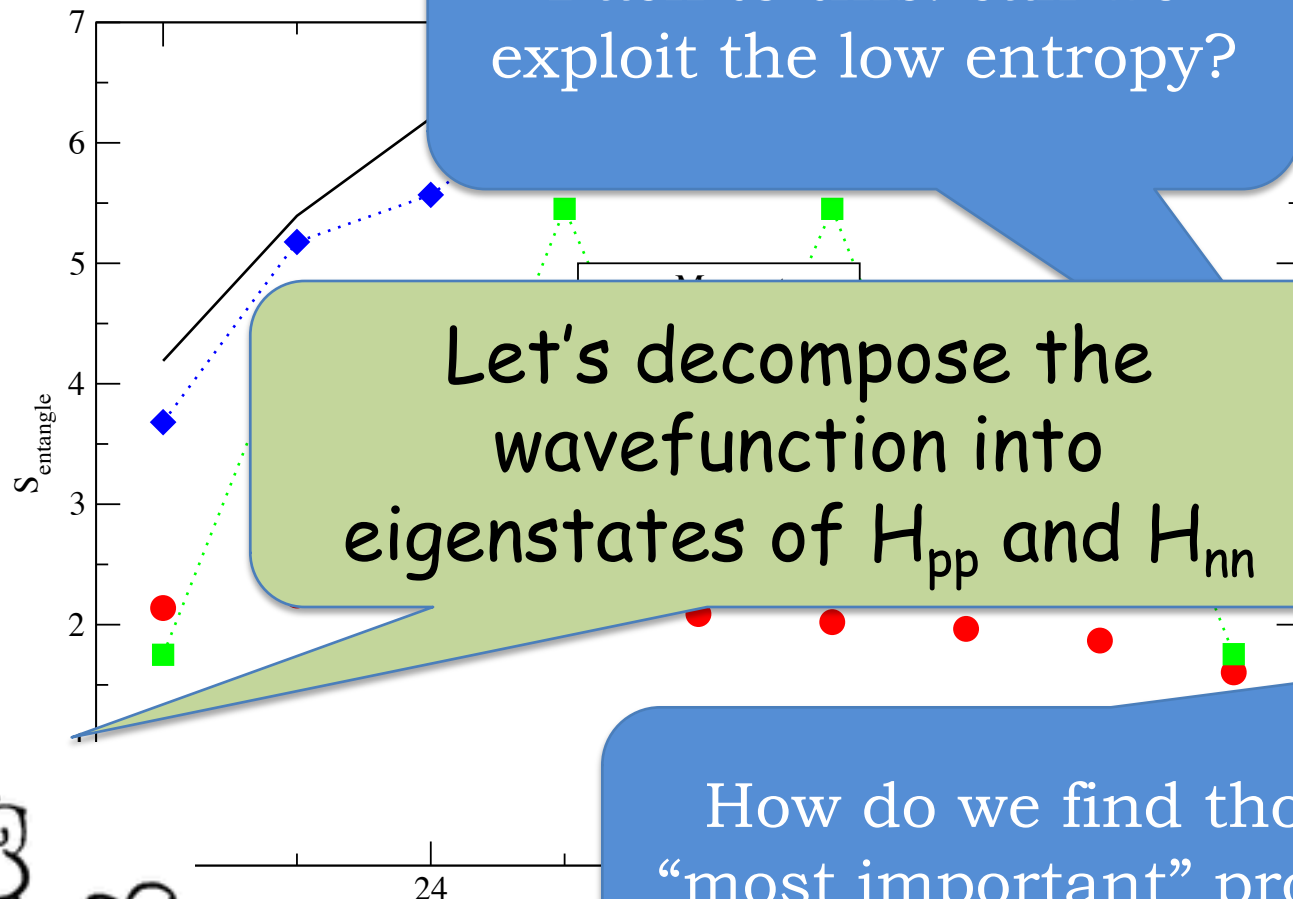


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Back to this: can we  
exploit the low entropy?



Z=N nuclei





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

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





This will test if we can use the  
*low-lying* eigenstates  
of  $H_{pp}$  and  $H_{nn}$  as building blocks

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

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





## Test:

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 
$$\mathbf{H}_{pp} \left| \Psi_p \right\rangle = E_p \left| \Psi_p \right\rangle \quad \mathbf{H}_{nn} \left| \Psi_n \right\rangle = E_n \left| \Psi_n \right\rangle$$

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





Test:

Solve

I can do this efficiently using  
the "Lanczos trick"

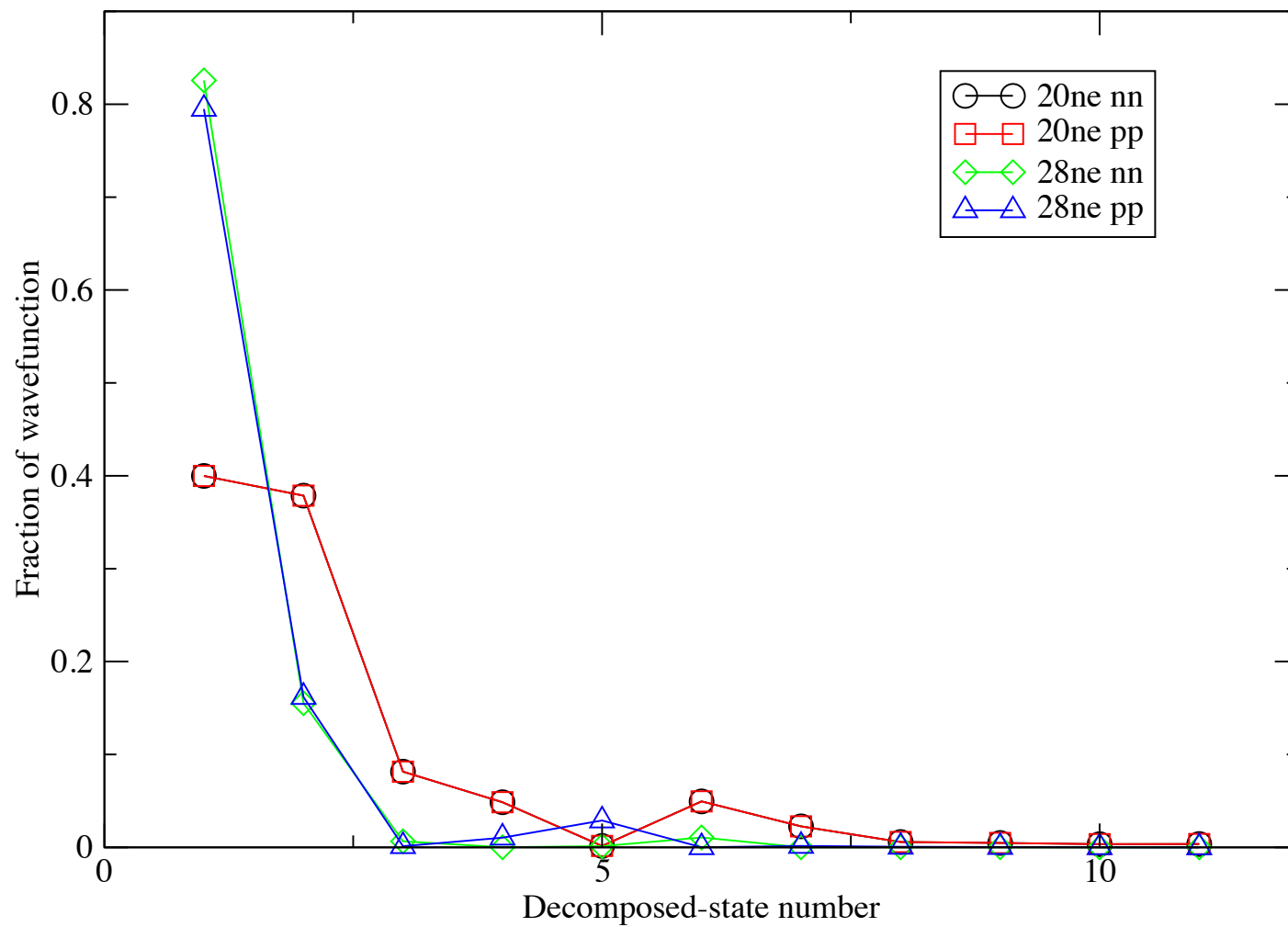
then solve

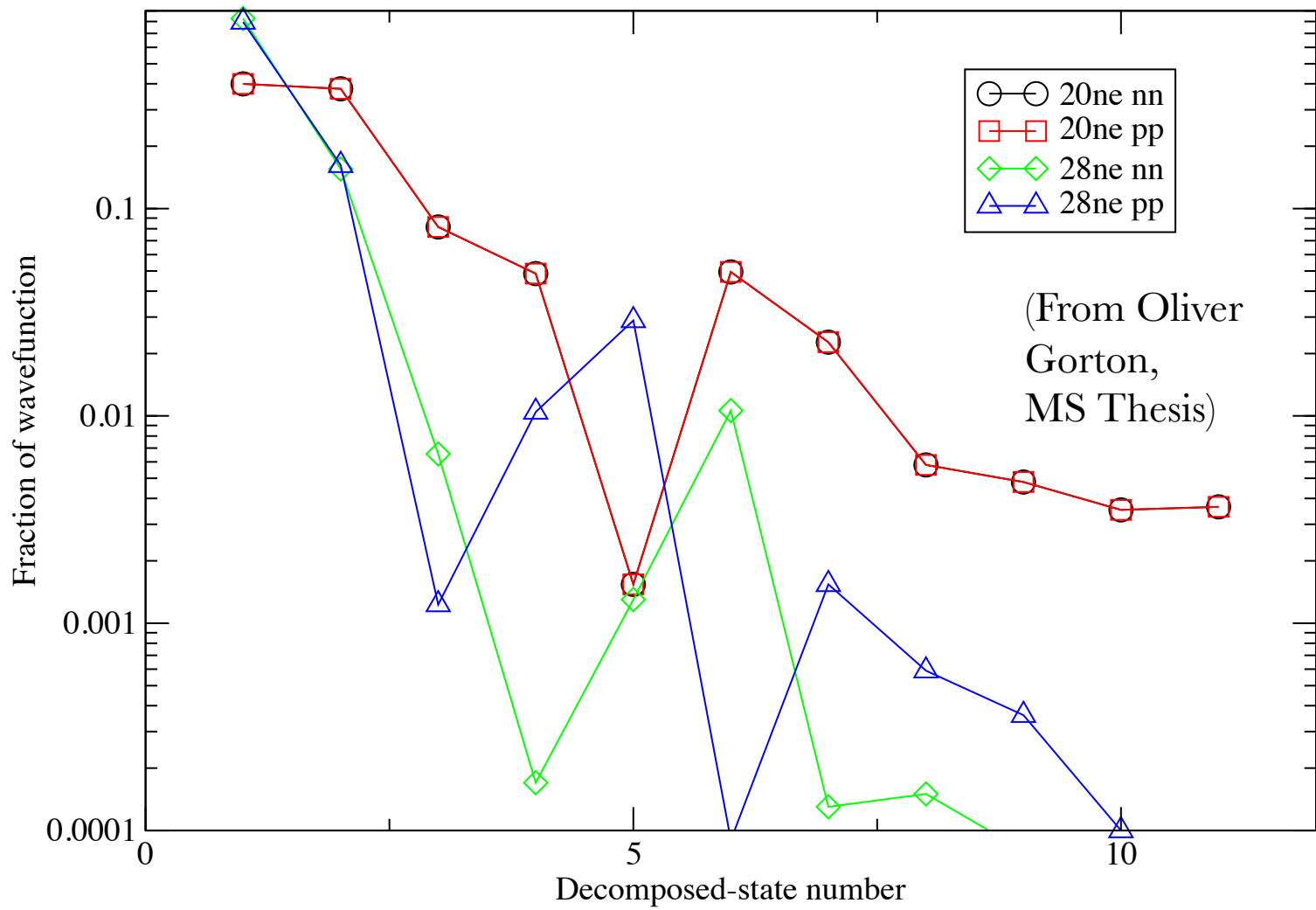
Expand

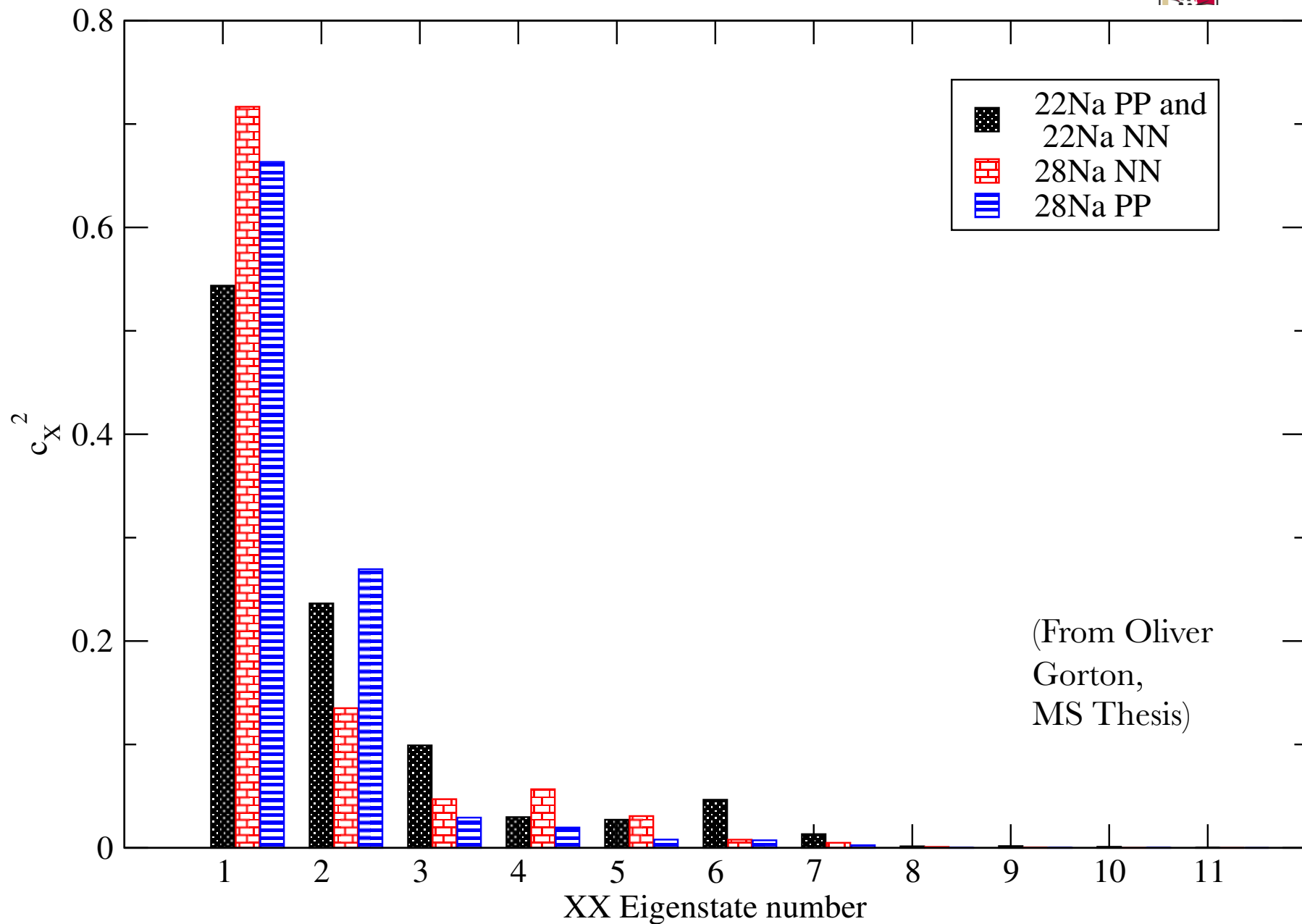
$$|\Psi_{full}\rangle = \sum_{p,n} c_{p,n} |\Psi_p\rangle \otimes |\Psi_n\rangle$$



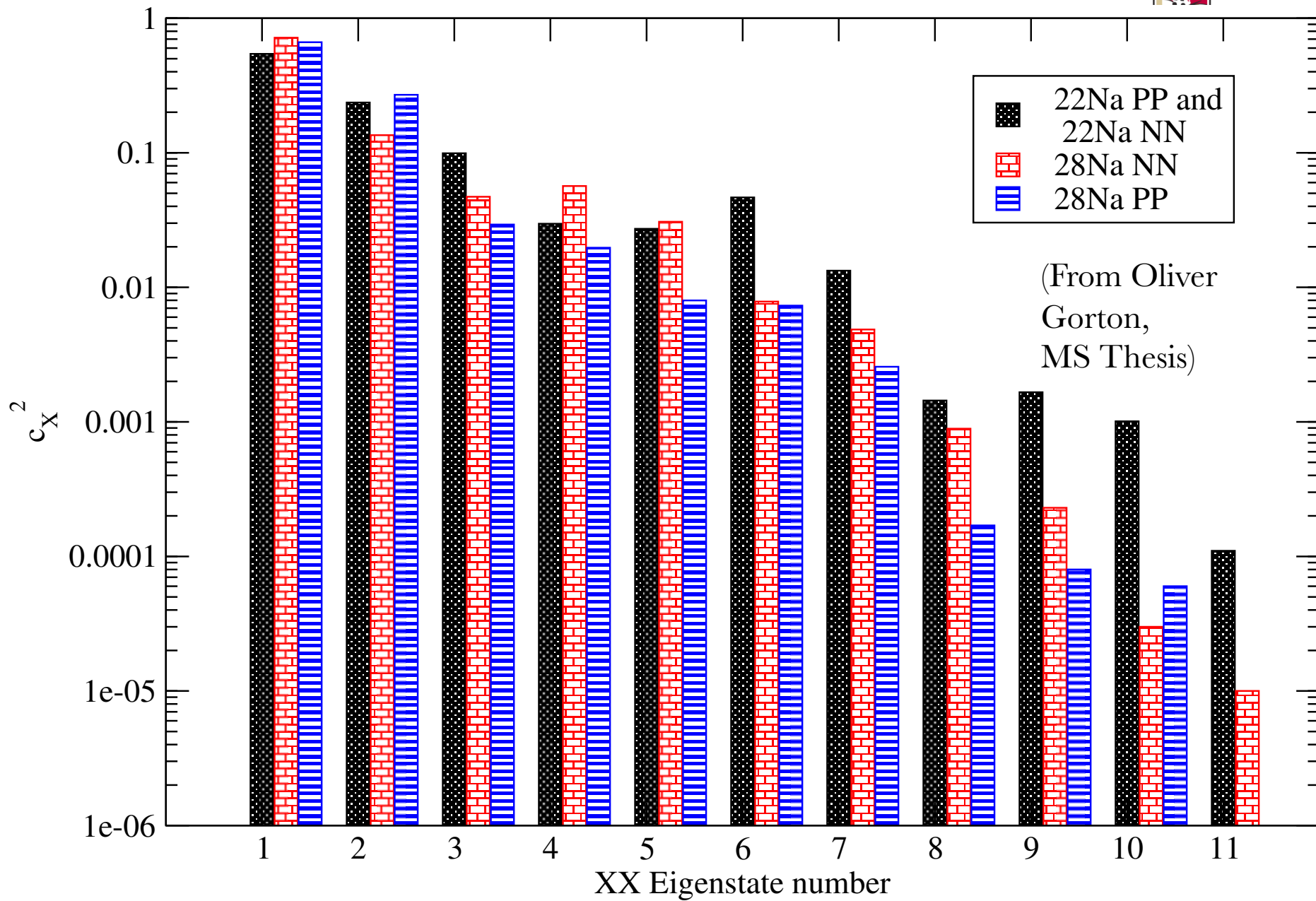
$$\text{compute } P(p) = \left| \langle \Psi_p | \Psi_{full} \rangle \right|^2 = \sum_n c_{p,n}^2$$







(From Oliver Gorton, MS Thesis)





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

We want to find solutions to

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

$$\text{We solve } \hat{H}_{pp}|\Psi_p\rangle = E_p|\Psi_p\rangle \quad \hat{H}_{nn}|\Psi_n\rangle = E_n|\Psi_n\rangle$$

and choose certain  $|\Psi_p\rangle, |\Psi_n\rangle$  as basis for diagonalization;

our results with the entropy suggest we only need a few



**PNISM = *proton-neutron interacting shell model***

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

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and choose certain  $|\Psi_p\rangle, |\Psi_n\rangle$  as basis for diagonalization;

our results with the entropy suggest we only need a few



Although BIGSTICK is an M-scheme code

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

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

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

This is true even if only protons or only neutrons





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.



Some "J-scheme" codes,  
such as NuShell(X), do this,  
but including *all* states.

states of good J

$\mu$

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

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



matrix elements of the Hamiltonian in basis of  
states and diagonalize.



Some "J-scheme" codes,  
such as NuShell(X), do this,  
but including *all* states.

ates of good J

By truncating we hope to get  
approximate solutions  
in much larger spaces

and  
to

$$|\Psi_I\rangle = \sum_{p,n} \left[ \langle \Psi_p^{a,J_p} | \otimes \langle \Psi_n^{b,J_n} | \right] J$$



rix elements of the Hamiltonian in basis of  
and diagonalize.



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  $\langle a_p | c_i^\dagger c_j | a'_p \rangle$

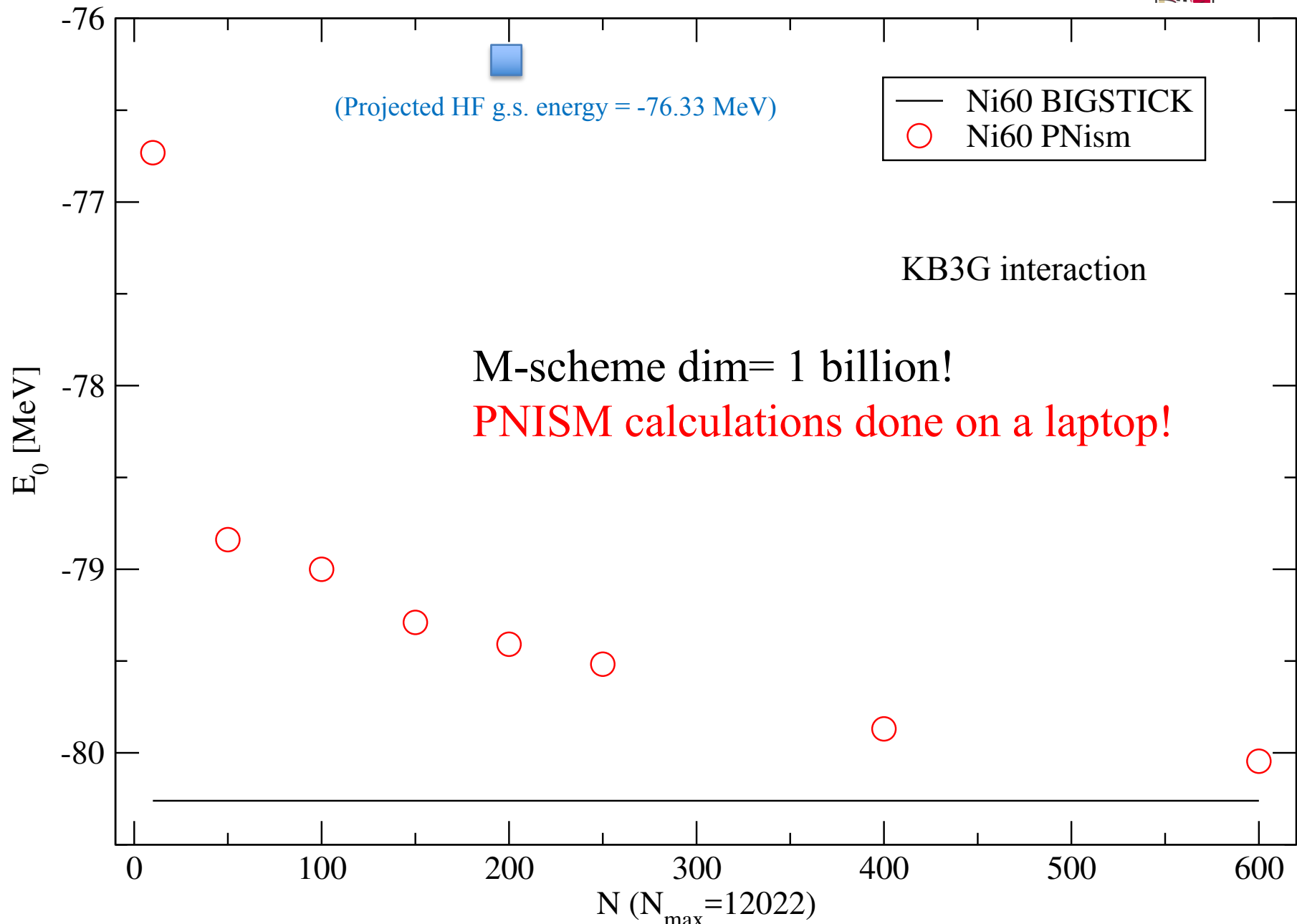
generate states  $|b_n\rangle$ , matrix elements  $\langle b_n | \mathbf{H}_{nn} | b'_n \rangle$   
and one body densities  $\langle b_n | c_i^\dagger c_j | b'_n \rangle$

PNISM (*proton-neutron interacting shell model*)

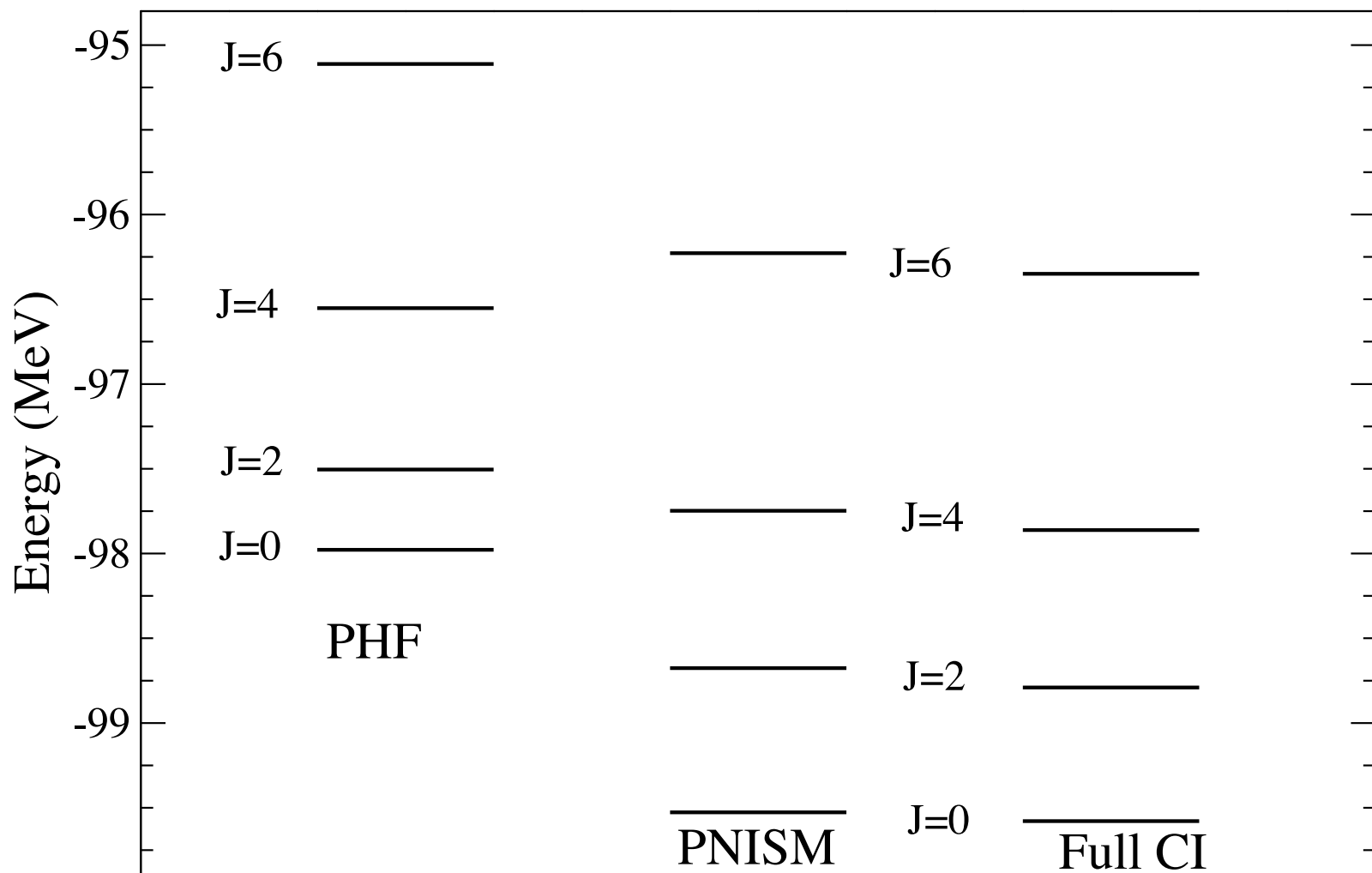
*read in the above and*

*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.

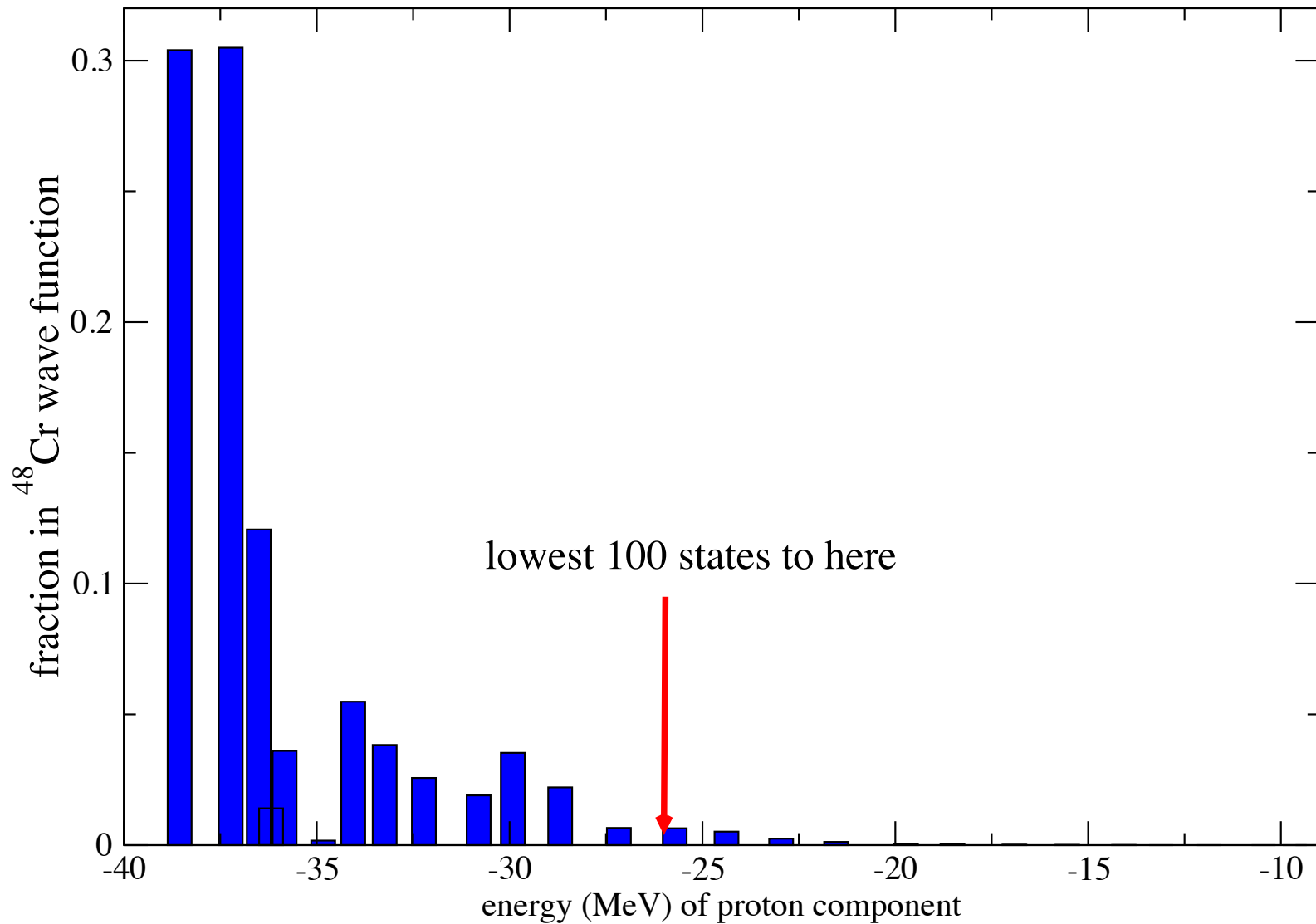


# $^{48}\text{Cr}$ , GX1A interaction



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

# $^{48}\text{Cr}$ , GX1A interaction





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

Sample application:

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

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

Proton dimension: 14,677

Neutron dimension: 646,430





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

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

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

Proton dimension = Neutron dimension = 3.7 million



# Summary:

- We can use *entanglement entropy* to see how “simple” a wave function looks in some bipartite basis.
- In many shell-model codes, it is natural to look at entanglement between neutron and proton Slater determinants
- With realistic interactions, shell model wave functions look simpler (have lower entropy) than with many schematic interactions (pairing, QQ)
- \* Entropy is often systematically lower for  $N \neq Z$



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This is not only enlightening,  
it is useful:

- Shell model codes are restricted in size of problem;  
how to go further?
- We build states using the “Weak-entanglement  
approximation” (WEA) for proton-neutron coupling.
- \* Looks promising—will try to apply to heavy nuclei



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Additional slides





It's also important to know:

Computational burden is *not* primarily the dimension but is the # of nonzero Hamiltonian matrix elements.

$$\sum_{\beta} H_{\alpha\beta} c_{\beta} = E c_{\alpha}$$



J-scheme matrices are smaller but much denser than M-scheme, and “symmetry-adapted” (i.e. SU(3)) matrices are smaller still.

example:  $^{12}\text{C}$   $N_{\text{max}} = 8$

scheme	basis dim	# of nonzero matrix elements
M	$0.6 \times 10^9$	$5 \times 10^{11}$
J (J=4)	$9 \times 10^7$	$3 \times 10^{13}$
SU(3)	$9 \times 10^6$	$2 \times 10^{12}$

(truncated)



It's also important to know:

Computational burden is *not* primarily the dimension but is the # of nonzero Hamiltonian matrix elements.

BIGSTICK's factorization algorithm is less efficient for  $N_{\max}$  calculations than for complete spaces.

e.g.  $^{51}\text{Cr}$  (dim 28 million) requires 0.4 Gb but

$^{12}\text{C}$   $N_{\max} = 6$  dim 30 million requires 6 Gb!

*to store the nonzero matrix elements would require  
~ 150 Gb!*



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Example of entanglement entropy:  
good angular momentum

Consider 2 spin-1/2 particles:

$$|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$$





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

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

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Example of entanglement entropy:  
good angular momentum

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

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

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

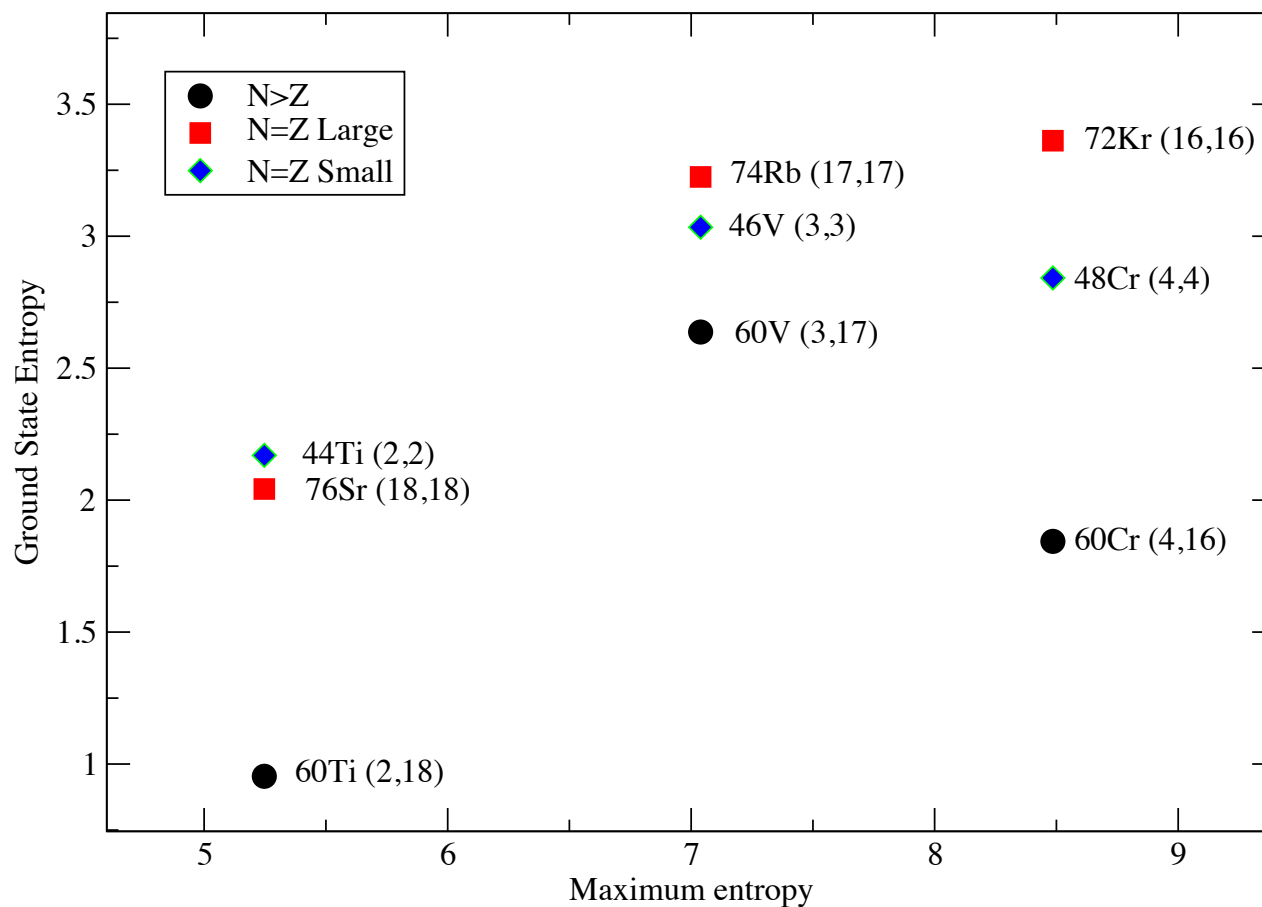
Note trace  $\rho = 1$ .



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## Entanglement entropy for ph conjugate triplets in the $^{40}\text{Ca}$ -core space

interaction file: gx1a



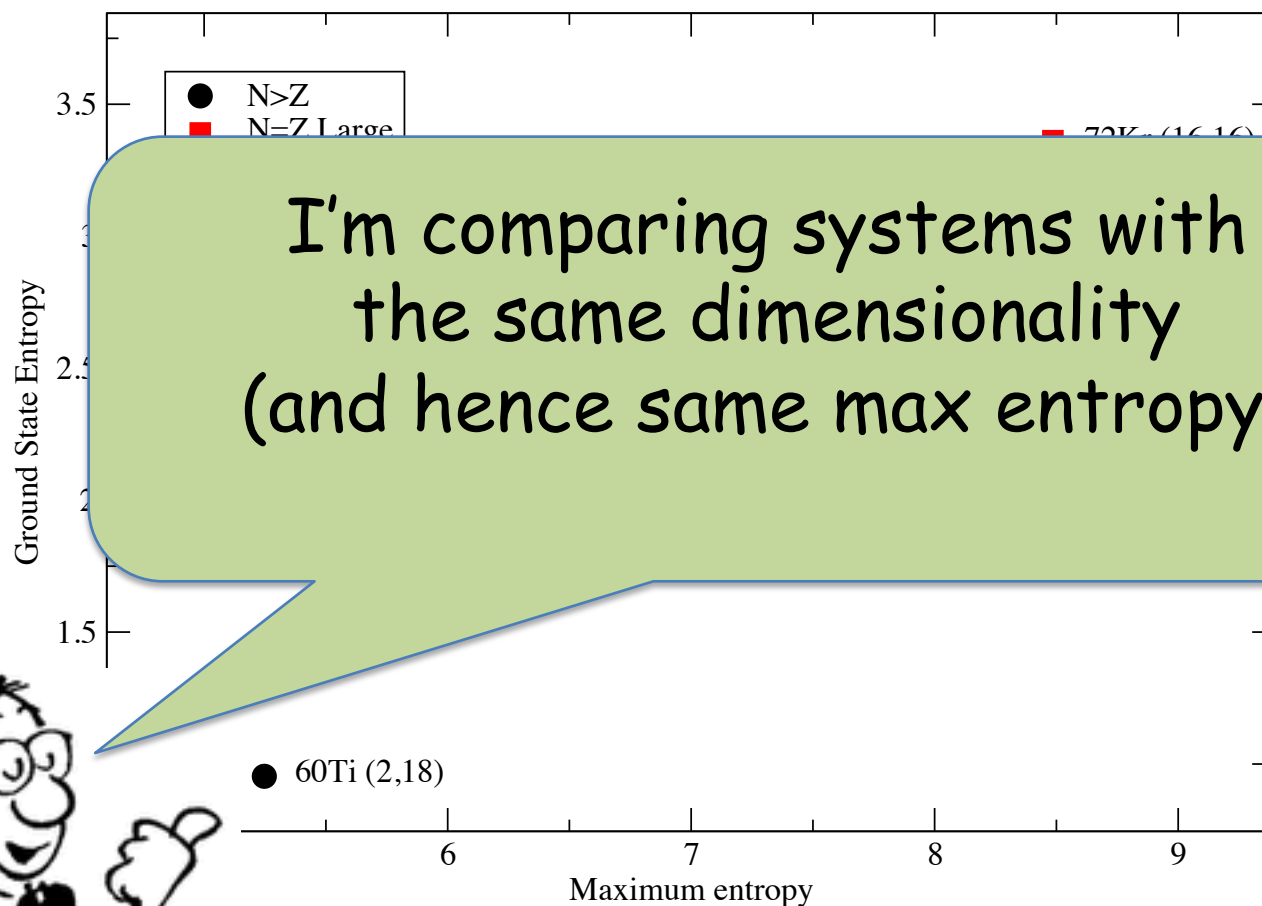
(From Oliver  
Gorton,  
MS Student)



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## Entanglement entropy for pn conjugate triplets in the $^{40}\text{Ca}$ -core space

interaction file: gx1a



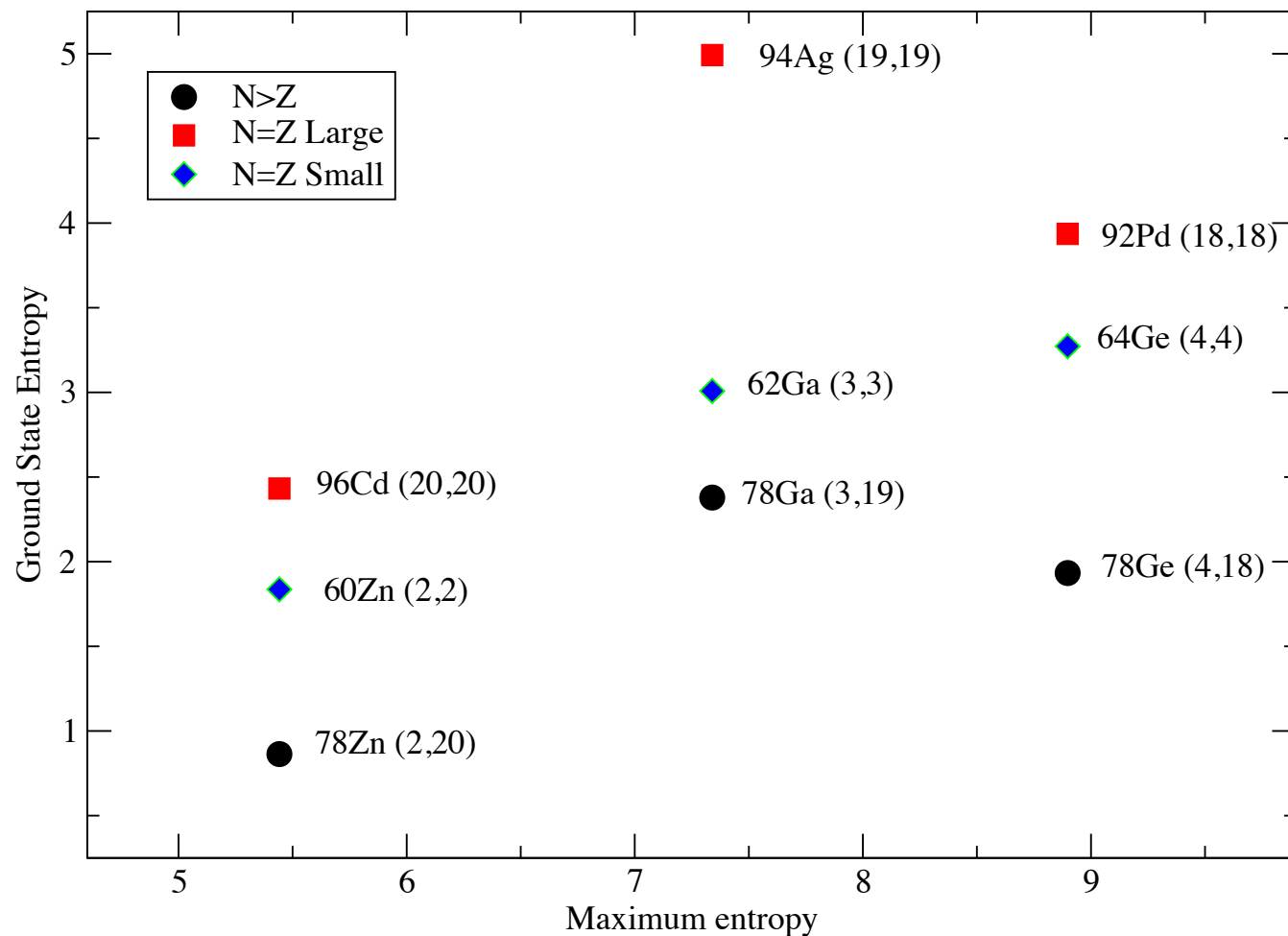
from Oliver  
Horton,  
(Student)





# Entanglement entropy for ph conjugate triplets in the $^{56}\text{Ni}$ -core space

interaction file: jun45



(From Oliver  
Gorton,  
MS Student)

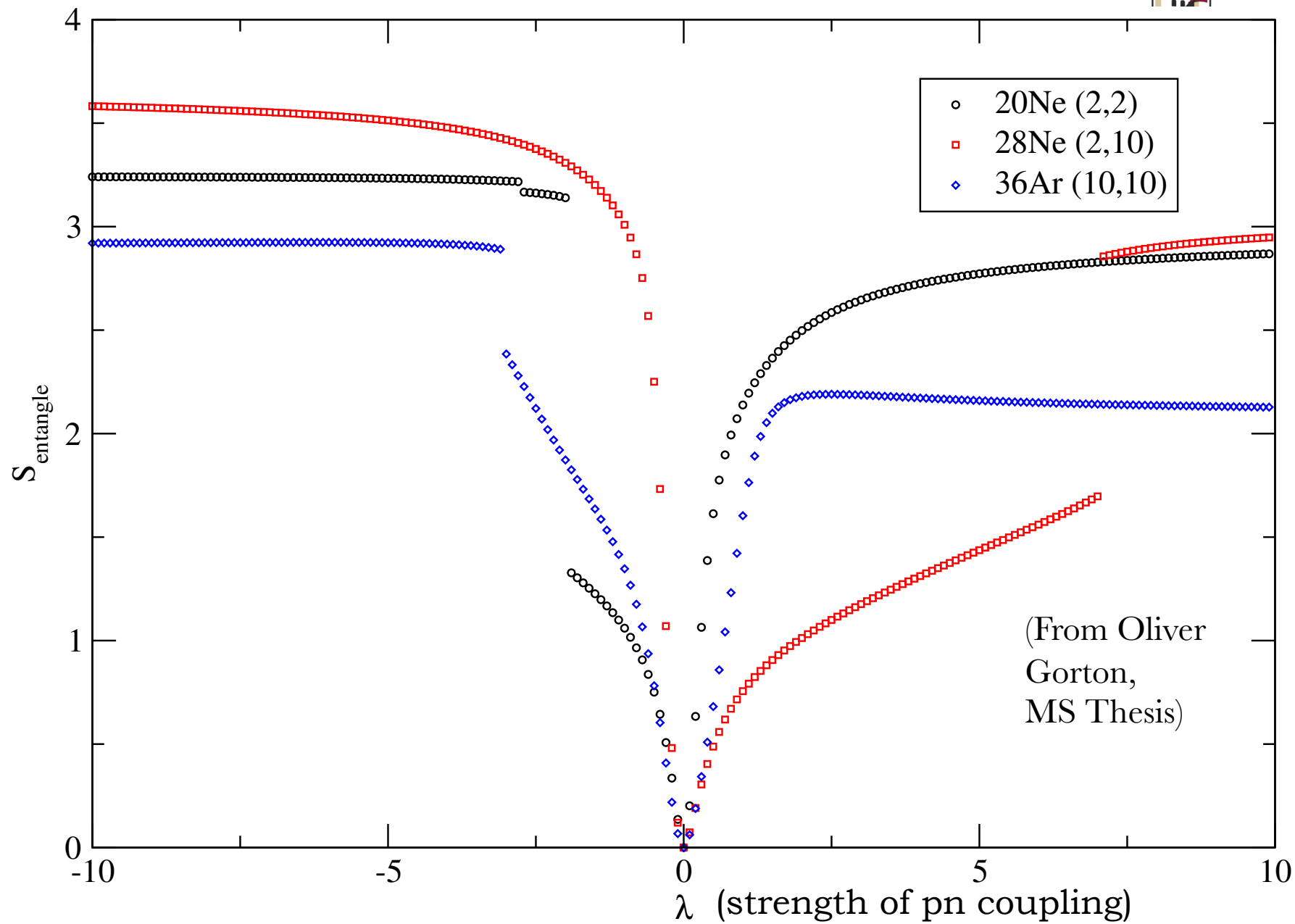


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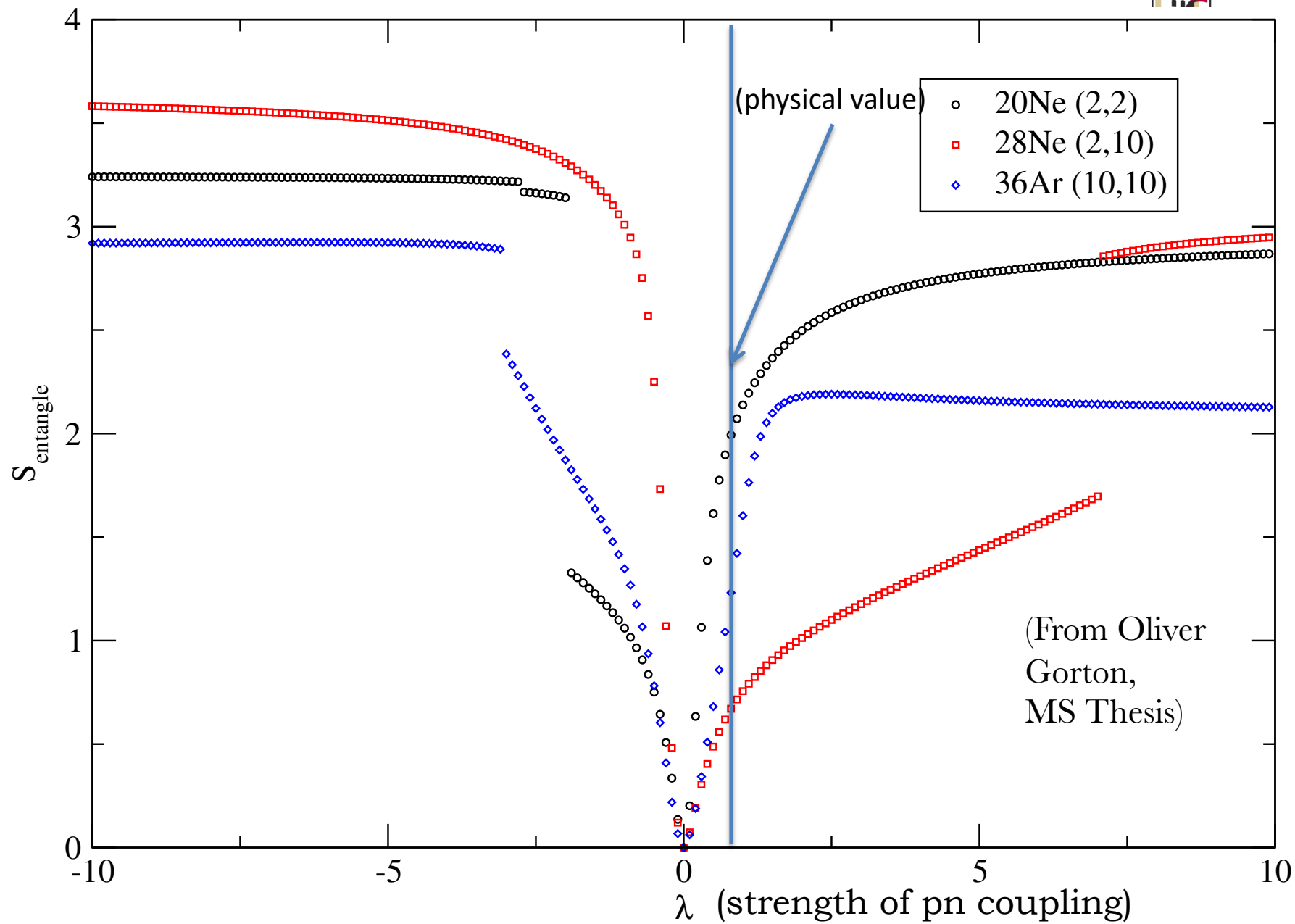
Let's see what happens as we change  
the strength of the  
proton-neutron coupling



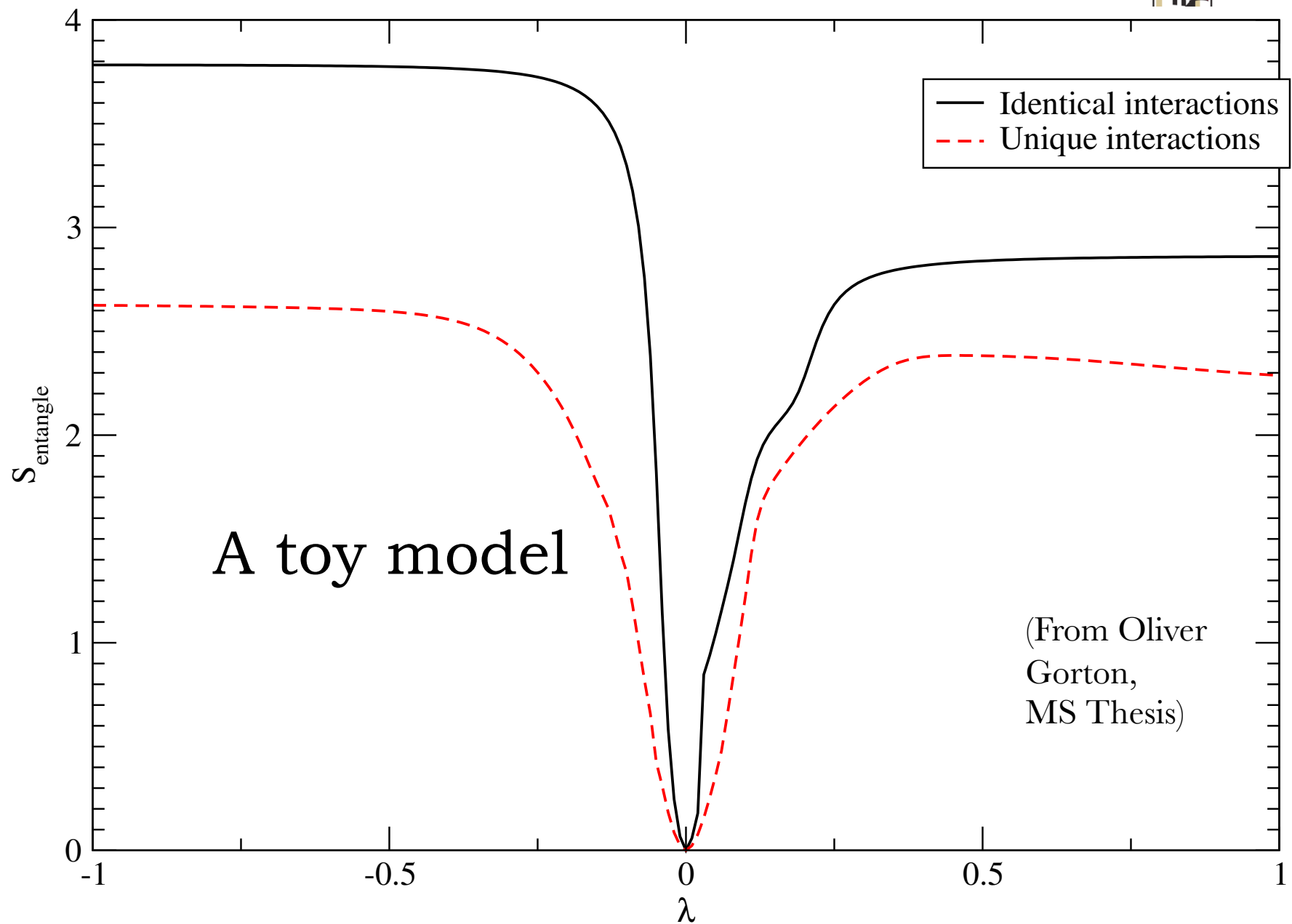




(From Oliver  
Gorton,  
MS Thesis)



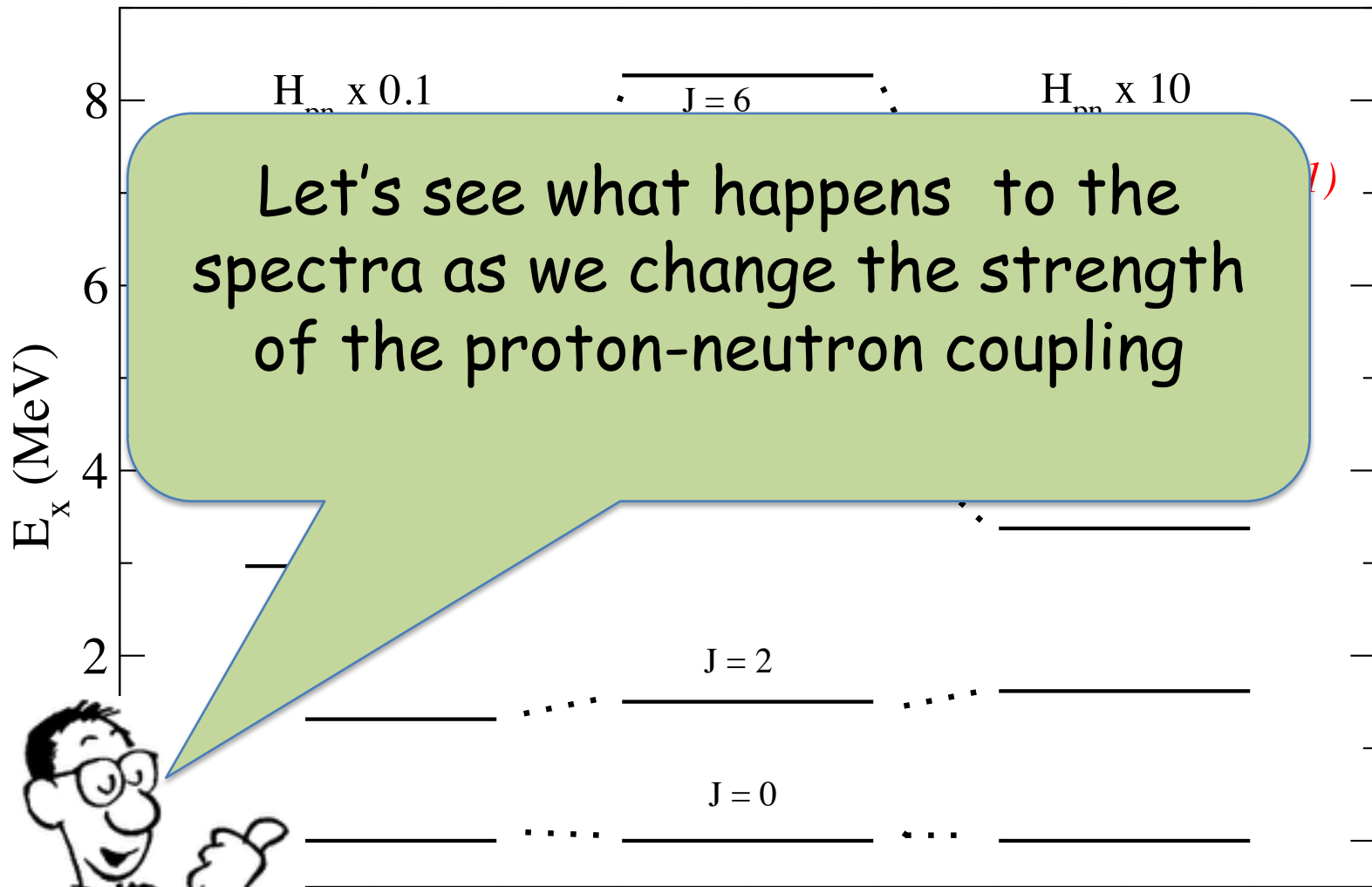
(From Oliver  
Gorton,  
MS Thesis)



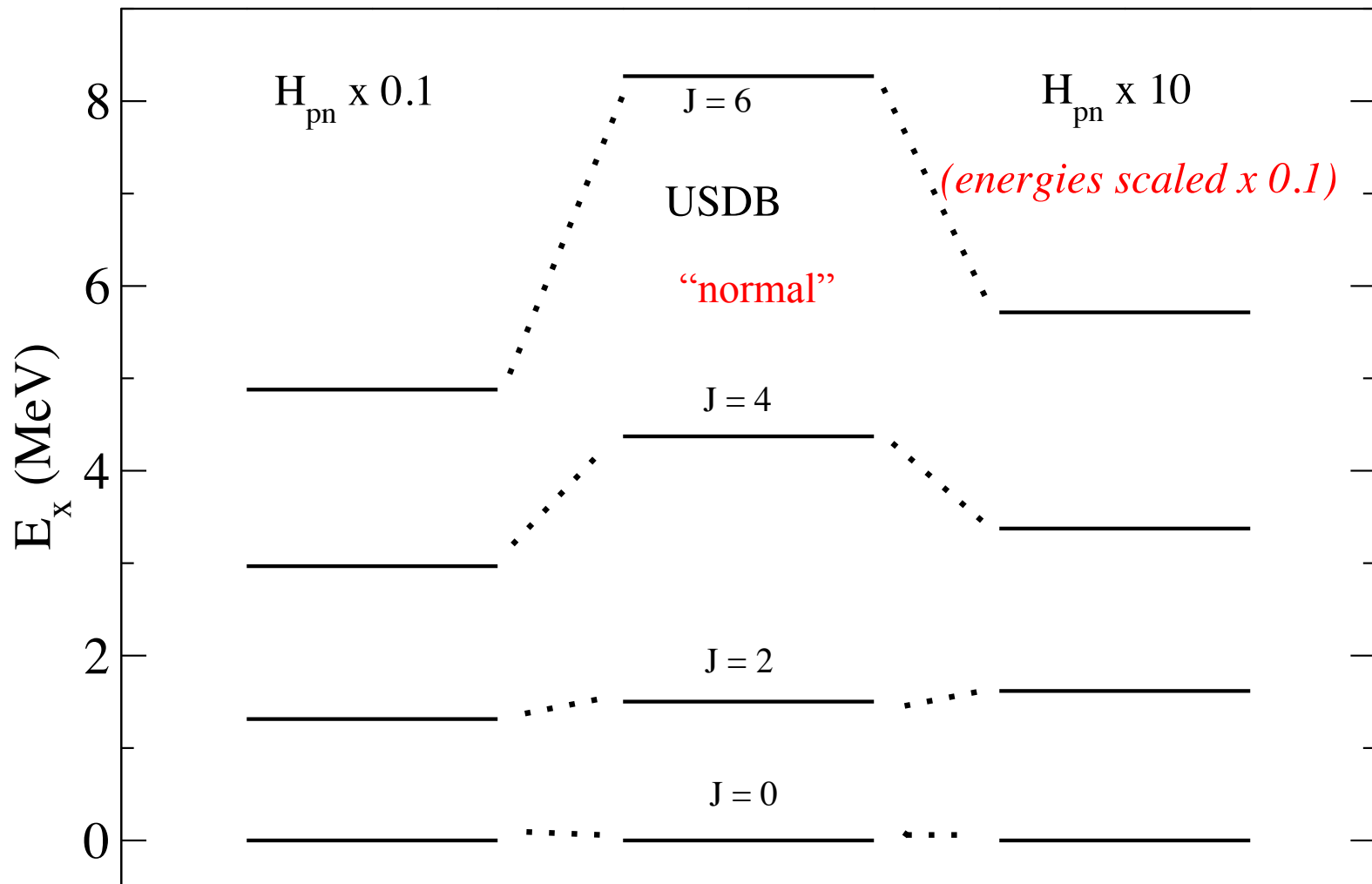
A toy model

(From Oliver  
Gorton,  
MS Thesis)

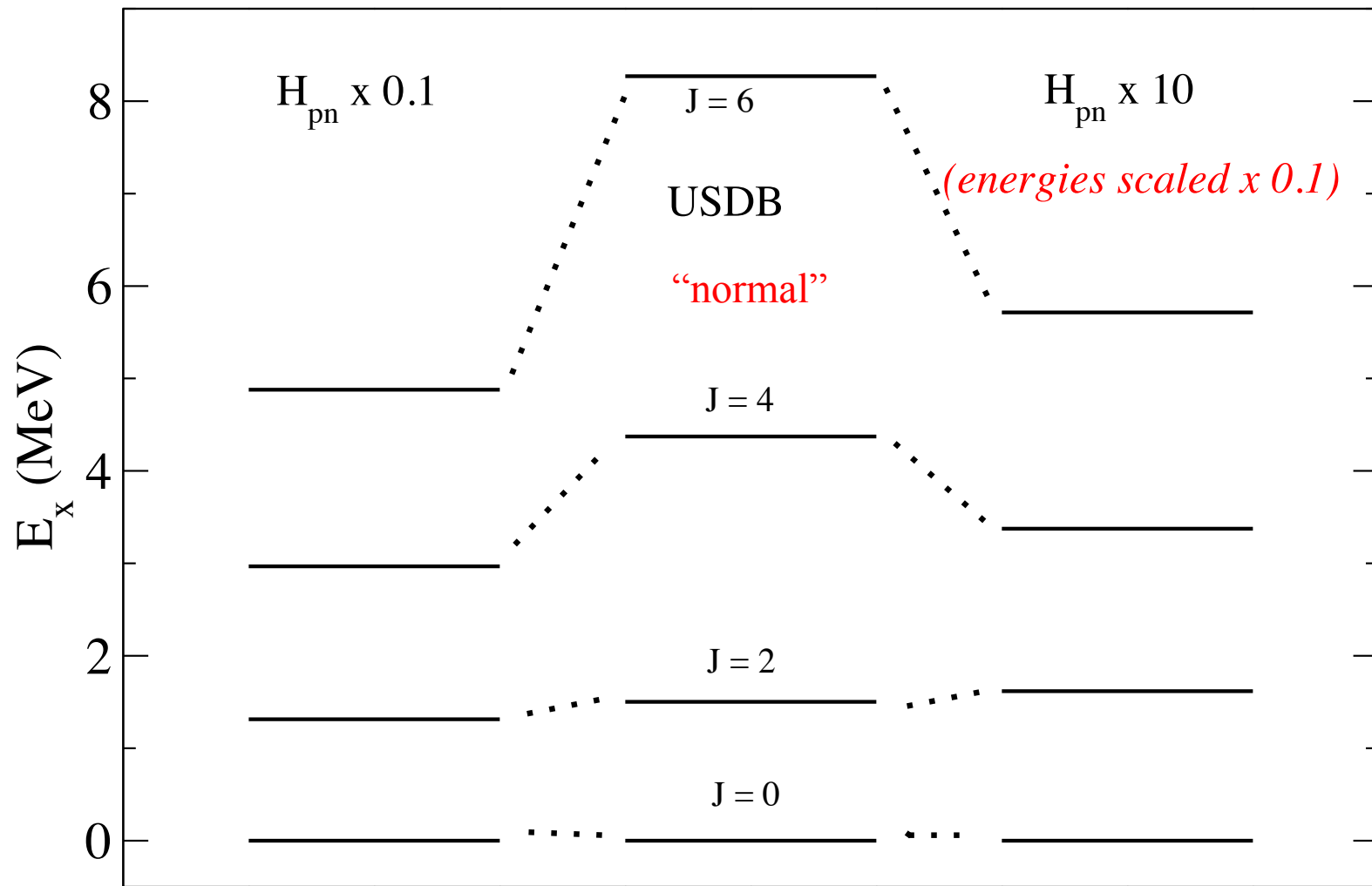
$^{24}\text{Mg}$



$^{24}\text{Mg}$



$^{24}\text{Mg}$



Overlap probability between states  $\sim 40\text{-}60\%$