# Disentangling nuclear wave functions

Calvin W. Johnson

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Expt. & Theo. Aspects of Neutron-Proton Pairing, Saclay, Sept 2023

## What do we need to describe atomic nuclei?

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What are the crucial degrees of freedom? i.e.,

- Deformation (single particles/mean-field)
- Pairing (S=0,T=1 and S=1,T=0 or *neutron-proton pairing)*
- Quartets/ 'alpha clusters'
- Other clusters?

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In other words, how do we *know* that quartets are more important than triplets?

# What do we need to describe
?

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We could look at *entanglement*

Isn't that just another word for 'correlations'?

gree

arti

S=1

*pairing)*

- Quartets/ 'alpha clusters
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# The difference between correlations and entanglement

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$$\hat{\rho} = |\Psi\rangle\langle\Psi|$$

and the *formal* density matrix

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In many-body theory we often introduce various density operators, such as the one-body density

$$\hat{c}_i^\dagger \hat{c}_j$$

and the two-body density

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BUT – these density operators and their matrices have different traces from the *formal* density matrix.

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$$tr \left\langle \hat{c}_i^\dagger \hat{c}_j \right\rangle = A$$

and

$$tr \left\langle \hat{c}_i^\dagger \hat{c}_j^\dagger \hat{c}_l \hat{c}_k \right\rangle = A(A-1)/2$$

in general, the trace of an *a*-body density is $\binom{A}{a} = \frac{A!}{a!(A-a)!}$.

The difference between the ‘formal’ density matrix and the *a*-body density matrices will be a challenge for us…..

back to 'formal' density matrices….

Next we define the *reduced* density matrix by tracing over one of the partitions:

$$|\Psi\rangle = \sum_{i,a} c_{i,a} \, |i\rangle \otimes |a\rangle \qquad \hat{\rho} = |\Psi\rangle\langle\Psi| \qquad \rho_{ia,jb} = c_{i,a} c^*_{j,b}$$

$$\rho^{red}_{i,j} = tr_a \rho = \sum_a c_{i,a} c^*_{j,a}$$

The reduced density matrix still has tr ρ = 1,

but is no longer necessarily idempotent: $\rho^2 \neq \rho$,

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If idempotent, the partitions are *not entangled*

but if *not* idempotent, the partitions are *entangled* back to ‘formal’ density matrices….

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but if *not* idempotent, the partitions are *entangled*

Looking at the eigenvalues of the reduced density matrix is related to **singular value decomposition** and is also called **Schmidt decomposition**

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Often one characterizes the eigenvalues by the *entanglement entropy:* $S = -\sum_n \lambda_n \ln \lambda_n$

(eigenvalues of $\rho^{red}$, $0 \leq \lambda_n \leq 1$ )

If the reduced density matrix has dimension $N$, then the maximum entropy is $S_{max} = \ln N$.

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# Early calculation of entanglement in nuclear systems:

O. Gorton MS thesis, 2018; CWJ and O. C. Gorton, J. Phys. G **50**, 045110 (2023)

The bipartite system was protons and neutrons, which works like a formal density matrix.

$$|\Psi\rangle = \sum_{i,a} c_{i,a} |p_i\rangle \otimes |n_a\rangle$$

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Here and throughout I calculate wave functions using configuration-interaction, expanding in an M-scheme (fixed total $J_z$) basis of shell-model Slater determinants.

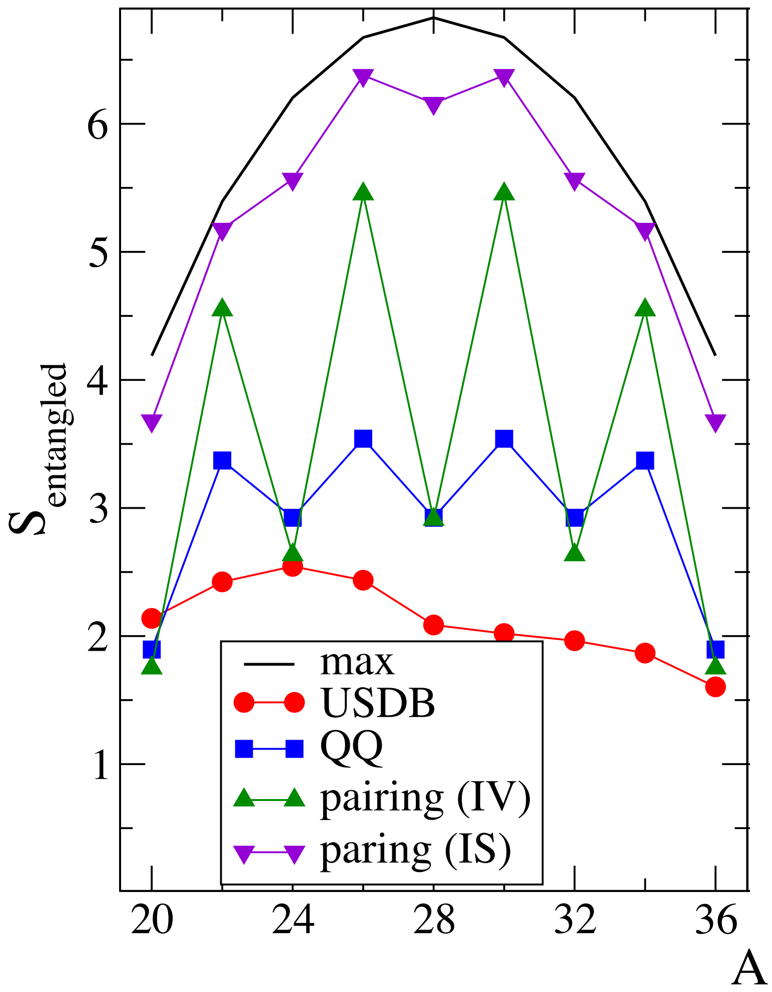
Here I also use empirical interactions, such as Brown & Richter's USDB interaction for the valence *sd* space (with frozen $^{16}O$ core).

In most shell-model codes, such as `Bigstick`, the basis already is bipartite in proton and neutron components, so carrying out such a decomposition is easy.

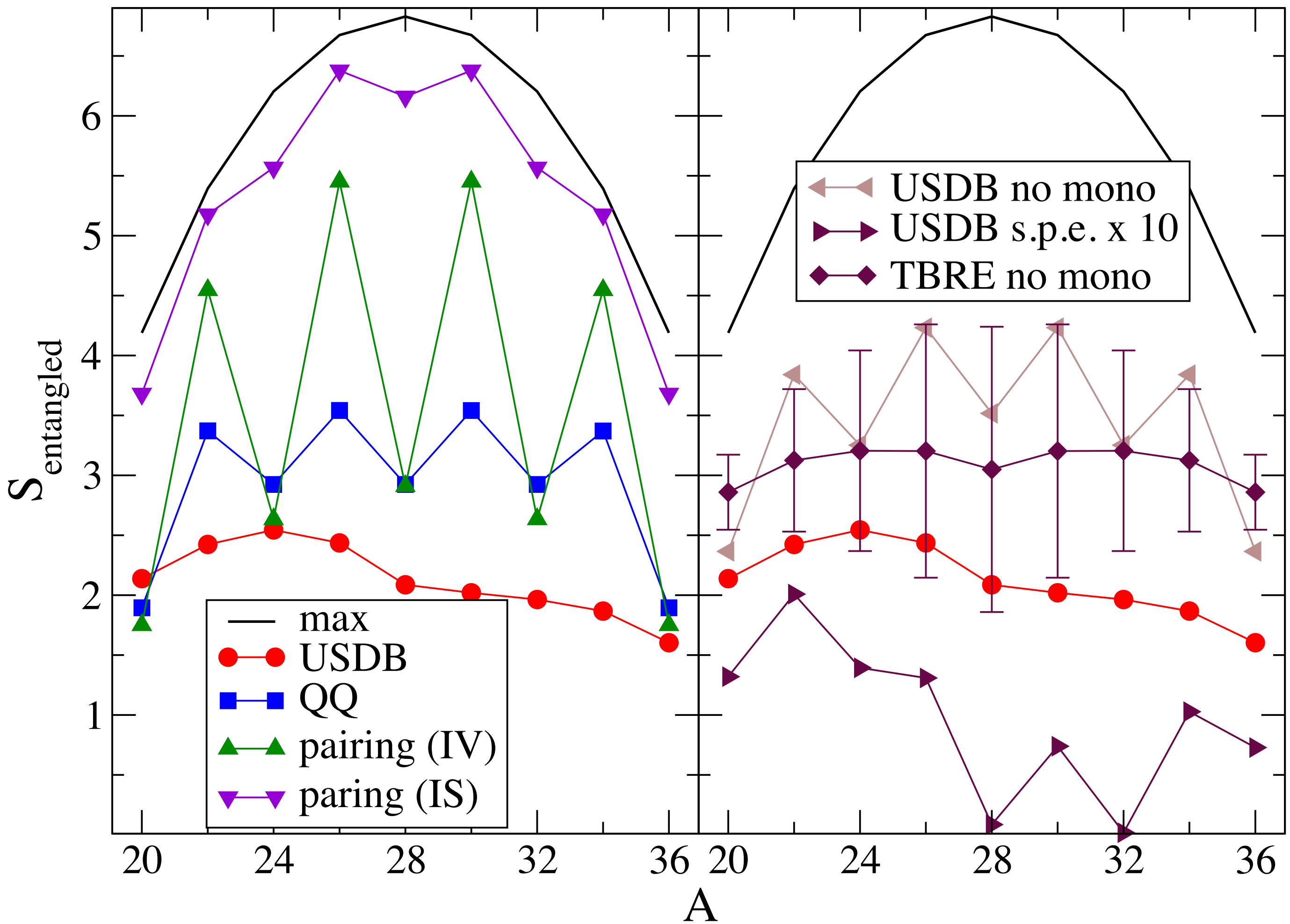
$$|\Psi\rangle = \sum_{i,a} c_{i,a} |p_i\rangle \otimes |n_a\rangle$$

can be extracted easily from `Bigstick` shell model code

Z = N nuclides in *sd* shell



Z = N nuclides in *sd* shell

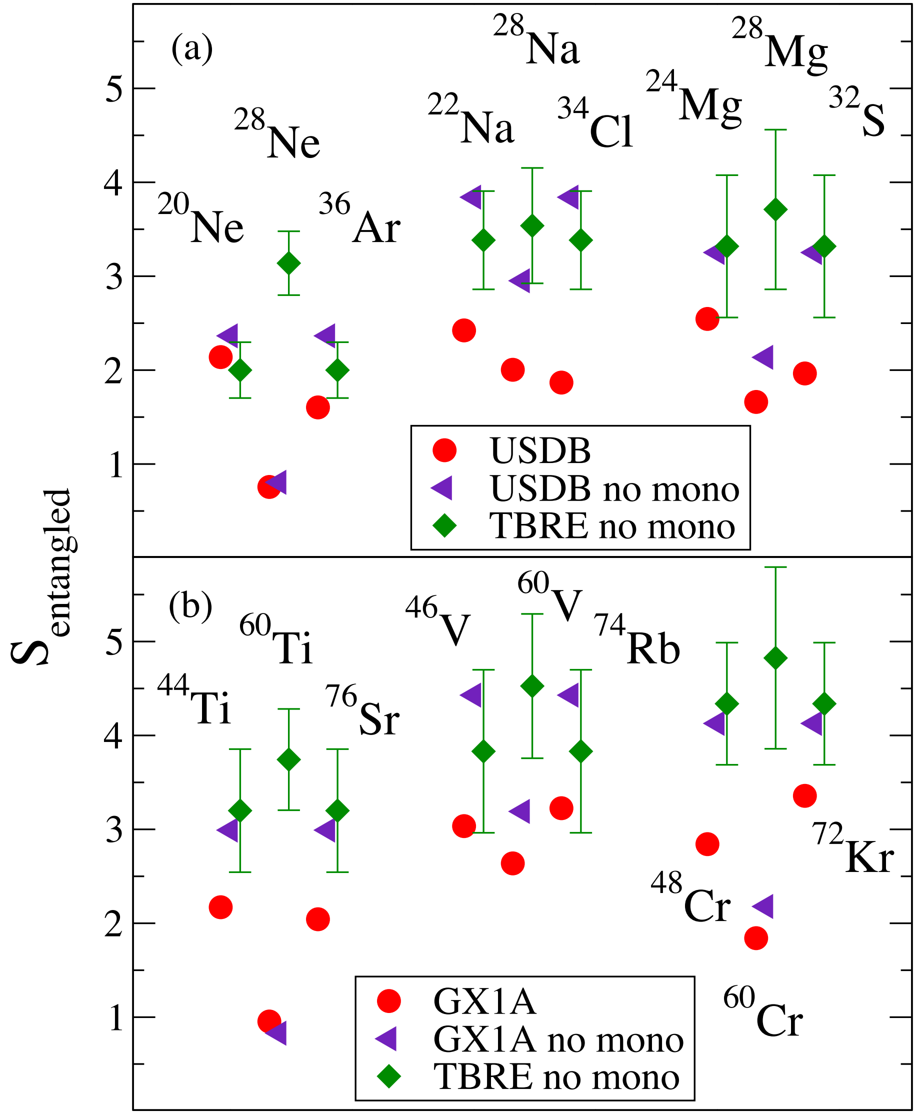


What we learn from this:

The shell structure (single-particle energies + monopole ($n^2$ terms), strongly affect the entropy,

and when you remove those terms, the entropies are similar to those from using *random* two-body interactions, at least for N = Z.

For N > Z (or < Z) we see interesting but unexplained patterns….


S_entangled
(a)
20Ne
28Ne
36Ar
22Na
28Na
34Cl
24Mg
28Mg
32S
USDB
USDB no mono
TBRE no mono
(b)
44Ti
60Ti
76Sr
46V
60V
74Rb
48Cr
60Cr
72Kr
GX1A
GX1A no mono
TBRE no mono

Expt

2023

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# Other related calculations:

Robin, Savage, and Pillet, Phys. Rev. C 103, 034325 (2021)

Use one- and two-nucleon entanglement to show that natural orbitals lead to decoupling of active and inactive spaces
(basically, a 'simpler' wave function)

A. Perez-Obiol, *et al*, arXiv:2307.05197

Calculates entanglement entropy with different slices of partitioning.
Z protons / N neutrons partitions (as in CWJ & Gorton) has lowest entropy.

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Can we use entanglement (or lack thereof) to signal important degrees of freedom?

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Entanglement measures how 'independent' a partition of a space is.

So, naively, one might imagine **dominant** degrees of freedom might have significantly smaller entanglement (or significantly larger)

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So let's compute the entanglement of 1, 2, 3, 4, … particles with the rest of the system. What pops out?

For instance, are two particles less entangled ('pairs') than three particles?

This is easier said than done.

Entanglement requires a bipartite basis

$$|\Psi\rangle = \sum_{i,a} c_{i,a} \, |i\rangle \otimes |a\rangle$$

However with *indistinguishable* particles, this can be tricky.
(Because of the different traces)

# We could normalize the *a*-body density matrices (so trace =1), *but:*

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A single Slater determinant would have nontrivial eigenvalues, which implies entanglement.

If we keep the combinatoric normalization, however, a single Slater determinant has **zero** entanglement entropy for any *a*-body correlations.

This latter makes sense because, intuitively, one would argue that, in second quantization, a single Slater determinant partitions trivially:

$$c_1^\dagger c_2^\dagger \, c_3^\dagger \,\big|\, c_4^\dagger c_5^\dagger c_6^\dagger |0\rangle$$

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Even keeping the combinatoric trace, how do we compare the results?

One way would be to compute $S/S_{max}$

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One way would be to compute $S/S_{max}$

How to do this:

1. Solve $\hat{H}|\Psi\rangle = E|\Psi\rangle$ using shell model code
2. Compute $\rho_{abc..,rst} = \langle\Psi|\hat{c}_a^\dagger \hat{c}_b^\dagger \hat{c}_c^\dagger \ldots \hat{c}_t \hat{c}_s \hat{c}_r|\Psi\rangle$
3. Find eigenvalues $\lambda_n$ of $\rho$ (because density, $\lambda_n \geq 0$)
4. $S = -\sum_n \lambda_n \ln \lambda_n$

# $^{24}$Mg (valence *sd*)

ground state $S/S_{max}$

| cluster | USDB | USDB (no mono) | random |
|---|---|---|---|
| 2p | 0.782 | 0.933 | 0.926 |
| 1p,1n | 0.818 | 0.959 | 0.955 |
| 3p | 0.643 | 0.802 | 0.805 |
| 2p,1n | 0.733 | 0.886 | 0.886 |
| 4p | 0.410 | 0.543 | 0.557 |
| 3p,1n | 0.576 | 0.720 | 0.721 |
| 2p,2n | 0.643 | 0.751 | 0.753 |

# $^{28}$Si (valence *sd*)

ground state $S/S_{max}$

| cluster | USDB | USDB (no mono) | random |
|---|---|---|---|
| 2p | 0.698 | 0.977 | 0.970 |
| 1p,1n | 0.720 | 0.984 | 0.982 |
| 3p | 0.640 | 0.941 | 0.933 |
| 2p,1n | 0.681 | 0.961 | 0.963 |
| 4p | 0.556 | 0.874 | 0.859 |
| 3p,1n | 0.622 | 0.923 | 0.926 |
| 2p,2n | 0.646 | 0.933 | 0.944 |

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# $^{28}$Si (valence *sd*)

ground state $S/S_{max}$

| cluster | USDB | USDB (no mono) | USDB, s.p.e. x 10 |
|---|---|---|---|
| 2p | 0.698 | 0.977 | 0.0377 |
| 1p,1n | 0.720 | 0.984 | 0.0426 |
| 3p | 0.640 | 0.941 | 0.0320 |
| 2p,1n | 0.681 | 0.961 | 0.0355 |
| 4p | 0.556 | 0.874 | 0.0263 |
| 3p,1n | 0.622 | 0.923 | 0.0302 |
| 2p,2n | 0.646 | 0.933 | 0.0316 |

Almost a perfect single Slater determinant

Effect of shell structure on entropies

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# $^{32}$S (valence *sd*)

ground state $S/S_{max}$

| cluster | USDB | USDB (no mono) | random |
|---|---|---|---|
| 2p | 0.700 | 0.988 | 0.929 |
| 1p,1n | 0.716 | 0.991 | 0.939 |
| 3p | 0.659 | 0.973 | 0.904 |
| 2p,1n | 0.687 | 0.980 | 0.025 |
| 4p | 0.613 | 0.949 | 0.866 |
| 3p,1n | 0.648 | 0.963 | 0.900 |
| 2p,2n | 0.661 | 0.967 | 0.911 |

This doesn't show what we hoped for!
Should I give up?

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This doesn't show what we hoped for!
Should I give up?

Not yet!

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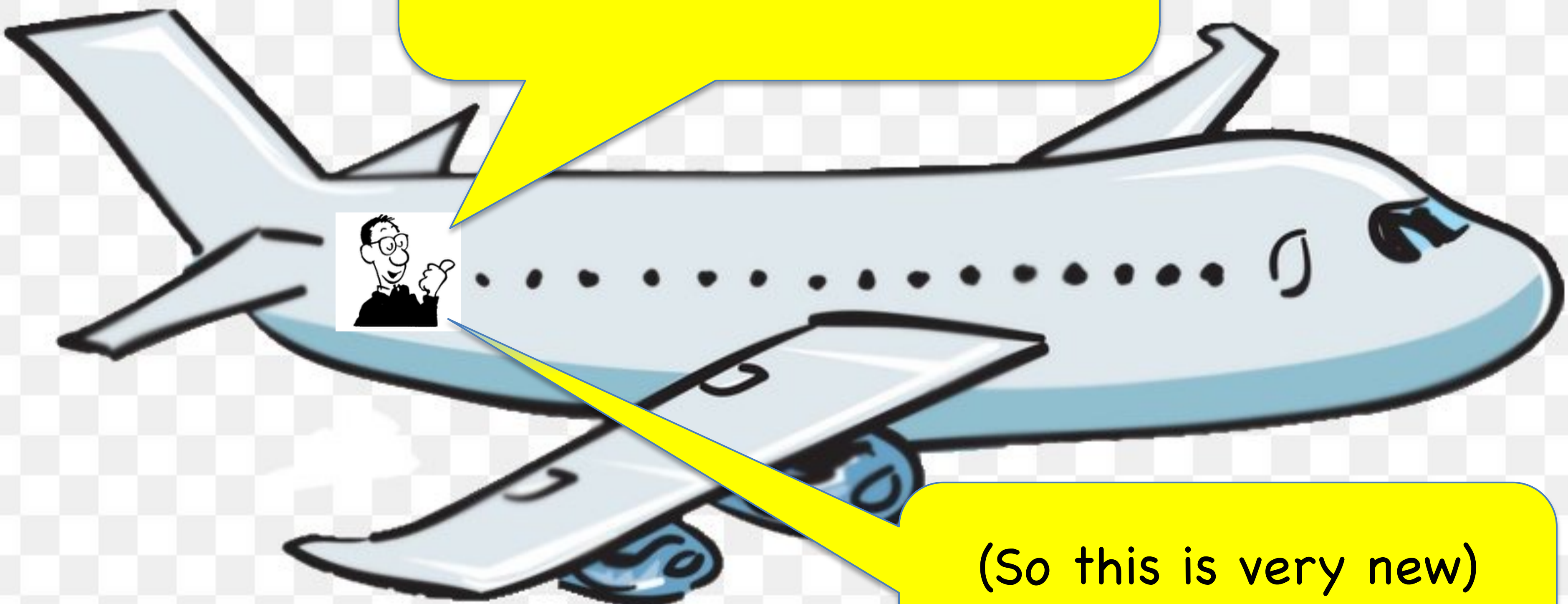
On the airplane ride here,
I remembered something…



(So this is very new)
(M. Savage recently
reminded me of this)

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Often one characterizes the eigenvalues by the *entanglement entropy:* $S = -\sum_n \lambda_n \ln \lambda_n$

(eigenvalues of $\rho^{\text{red}}$, $0 \leq \lambda_n \leq 1$ )

The entanglement entropy is convenient but blunt.

Sometimes one plots the *entanglement spectrum* which, traditionally, is $-\ln(\lambda_n)$

Li and Haldane, PRL **101**, 010504 (2008)

Small values ( = large $\lambda_n$) and 'gaps' in the spectrum are meaningful

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How to do this:

1. Solve $\hat{H}|\Psi\rangle = E|\Psi\rangle$ using shell model code
2. Compute $\rho_{abc..,rst} = \langle\Psi|\hat{c}_a^\dagger\hat{c}_b^\dagger\hat{c}_c^\dagger \ldots \hat{c}_t\hat{c}_s\hat{c}_r|\Psi\rangle$
3. Find eigenvalues $\lambda_n$ of $\rho$ (because density, 1? $\geq \lambda_n \geq 0$)
4. Plot $-\ln(\lambda_n)$

(also see Sambataro & Sandulescu, Ann. Phys. 413, 168061 (2020) and N. Sandulescu's talk from this workshop series, 2019)

In most of my calculations, I remove the shell structure (single-particle energies and monopole interactions) and compare to a randomly generated two-body interaction; the latter acts as a control.

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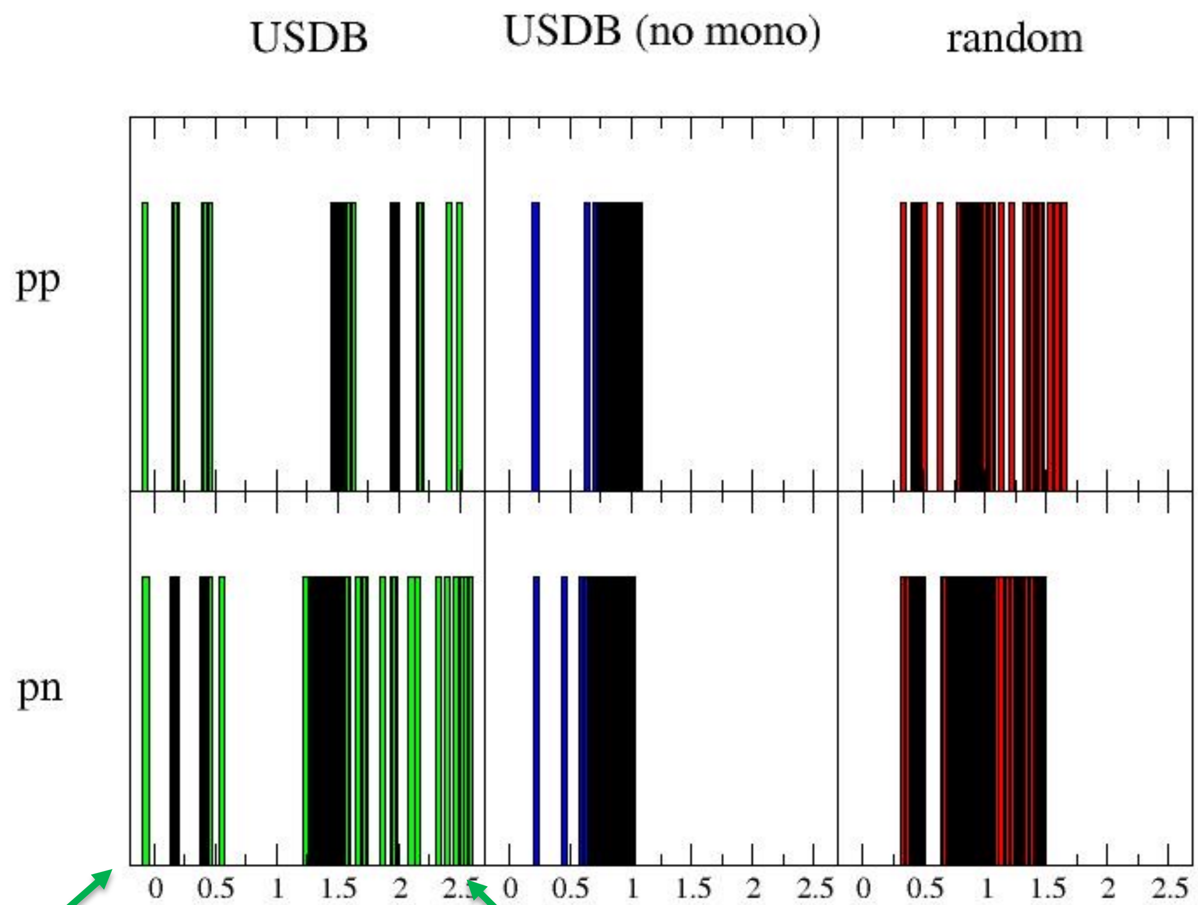


high correlation

low correlation

These have very similar entropies, but the spectra differ

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# $^{32}$S (valence *sd*)

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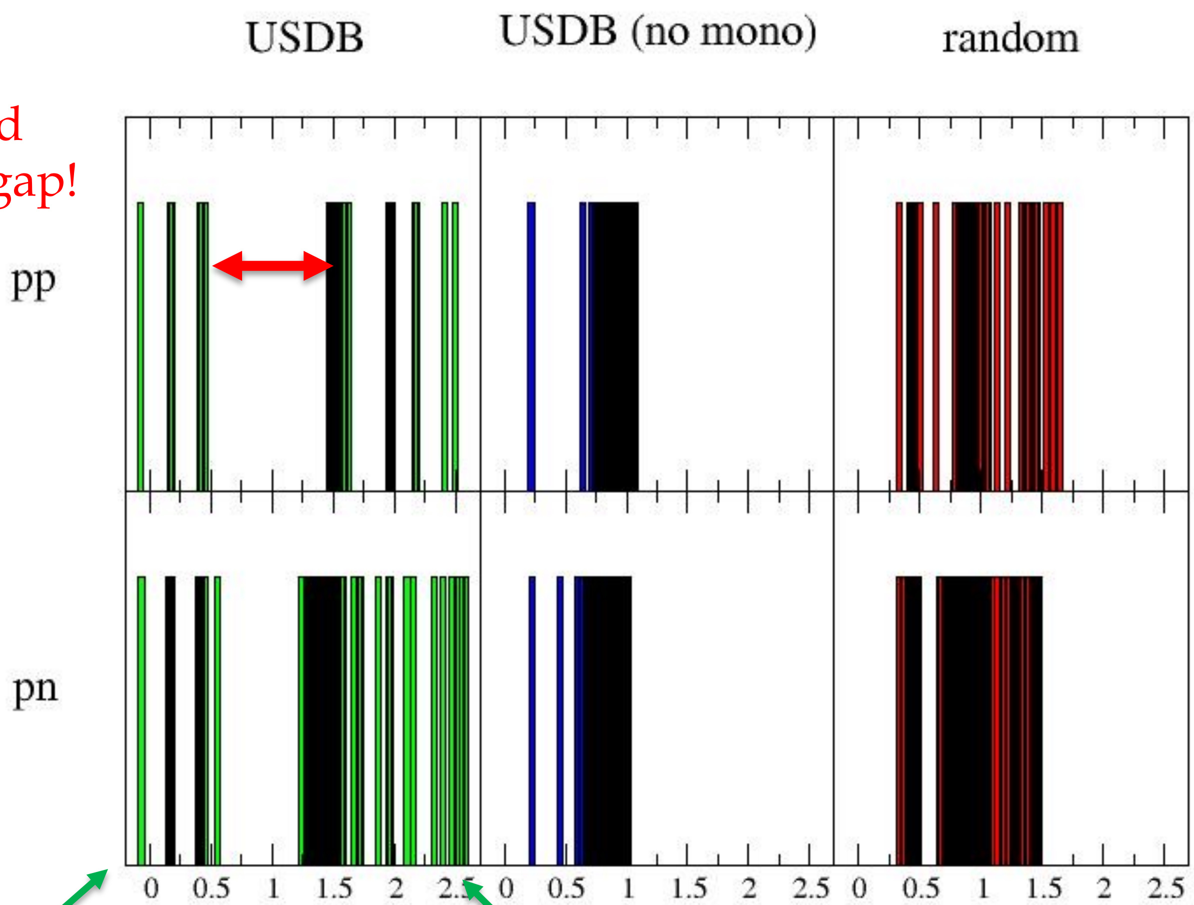
ground state $-\ln \lambda_n$




Mind the gap!

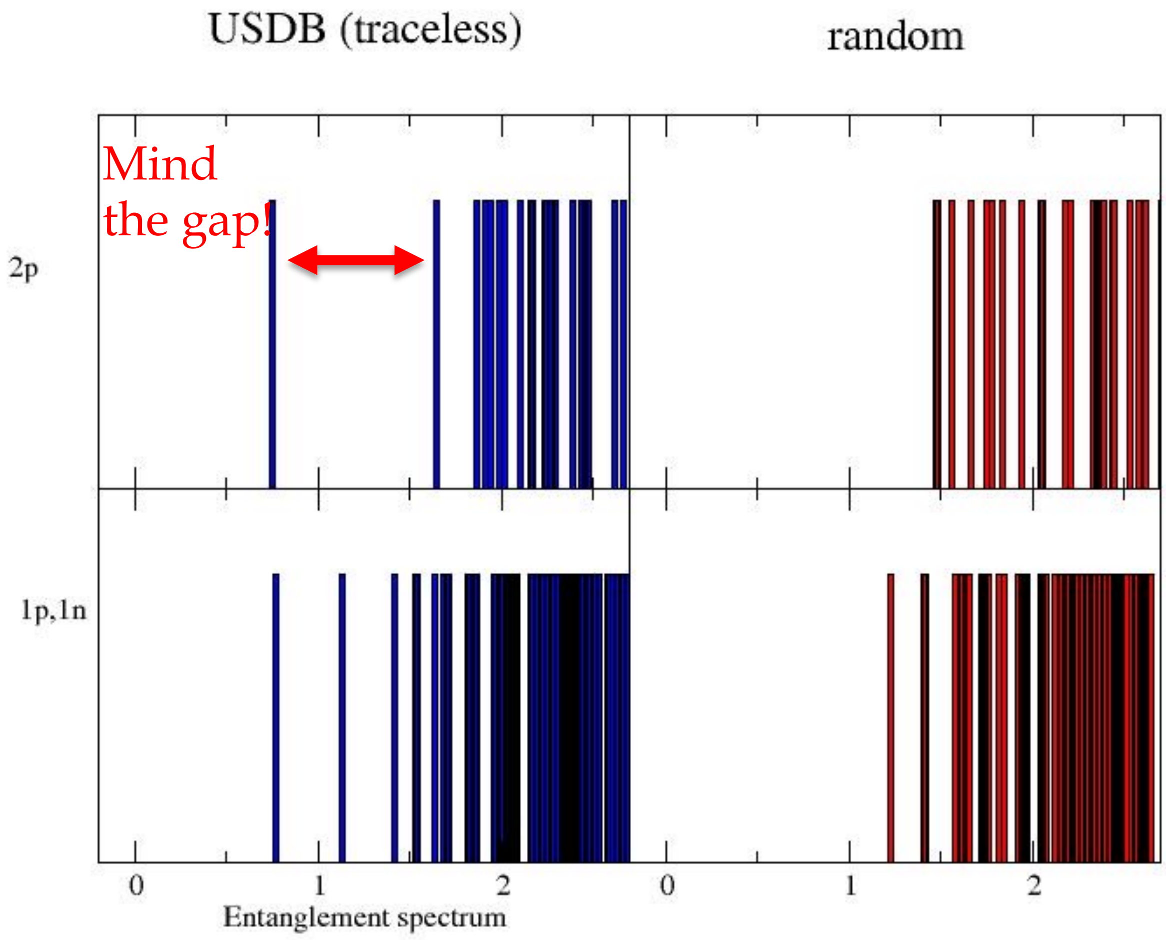
These have very similar entropies, but the spectra differ

high correlation

low correlation

# $^{24}$Mg (valence *sd*)

ground state $-\ln \lambda_n$

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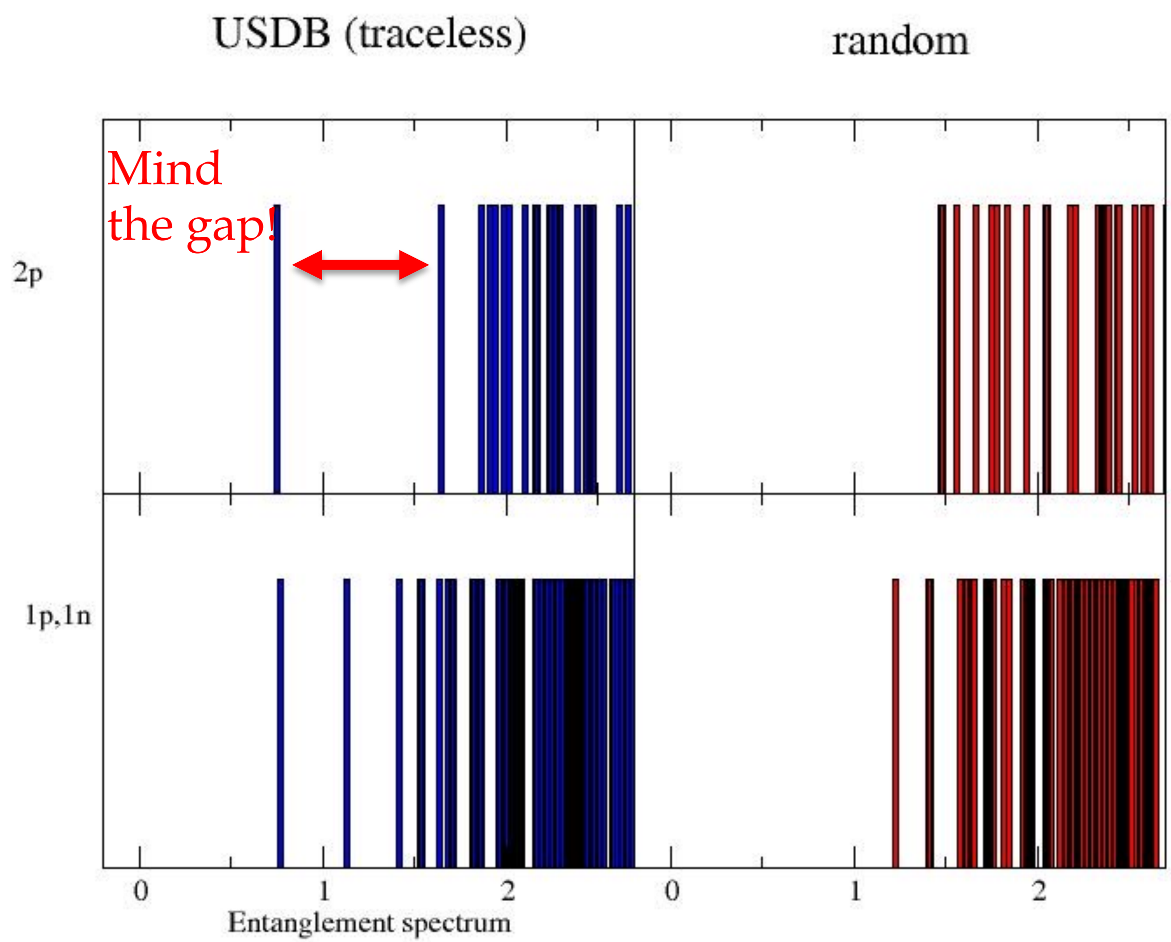


Note: these are not necessarily J = 0,1 pairs; the results are *agnostic*

These have very similar entropies, but the spectra differ

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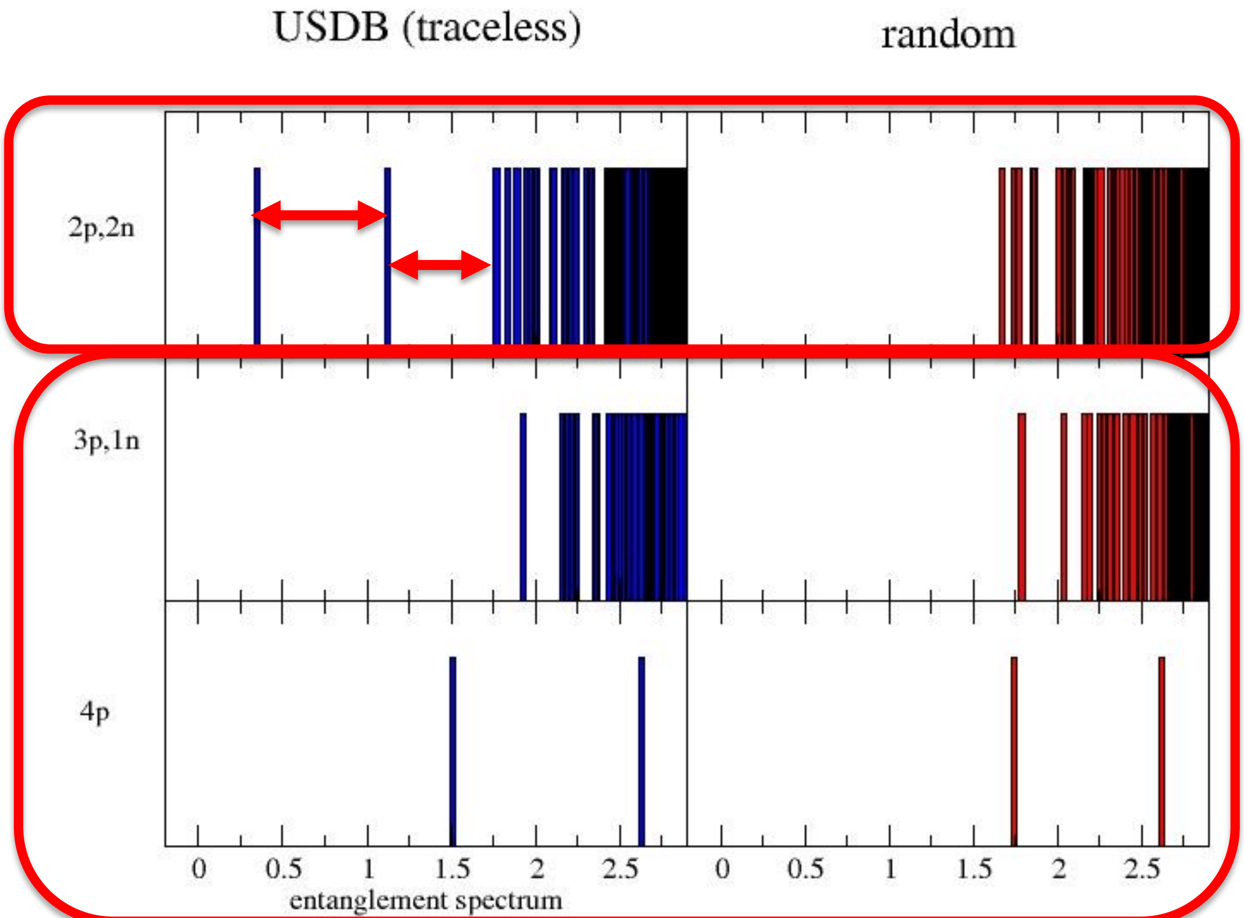


These have very similar entropies, but the spectra differ

…while these spectra are not very different

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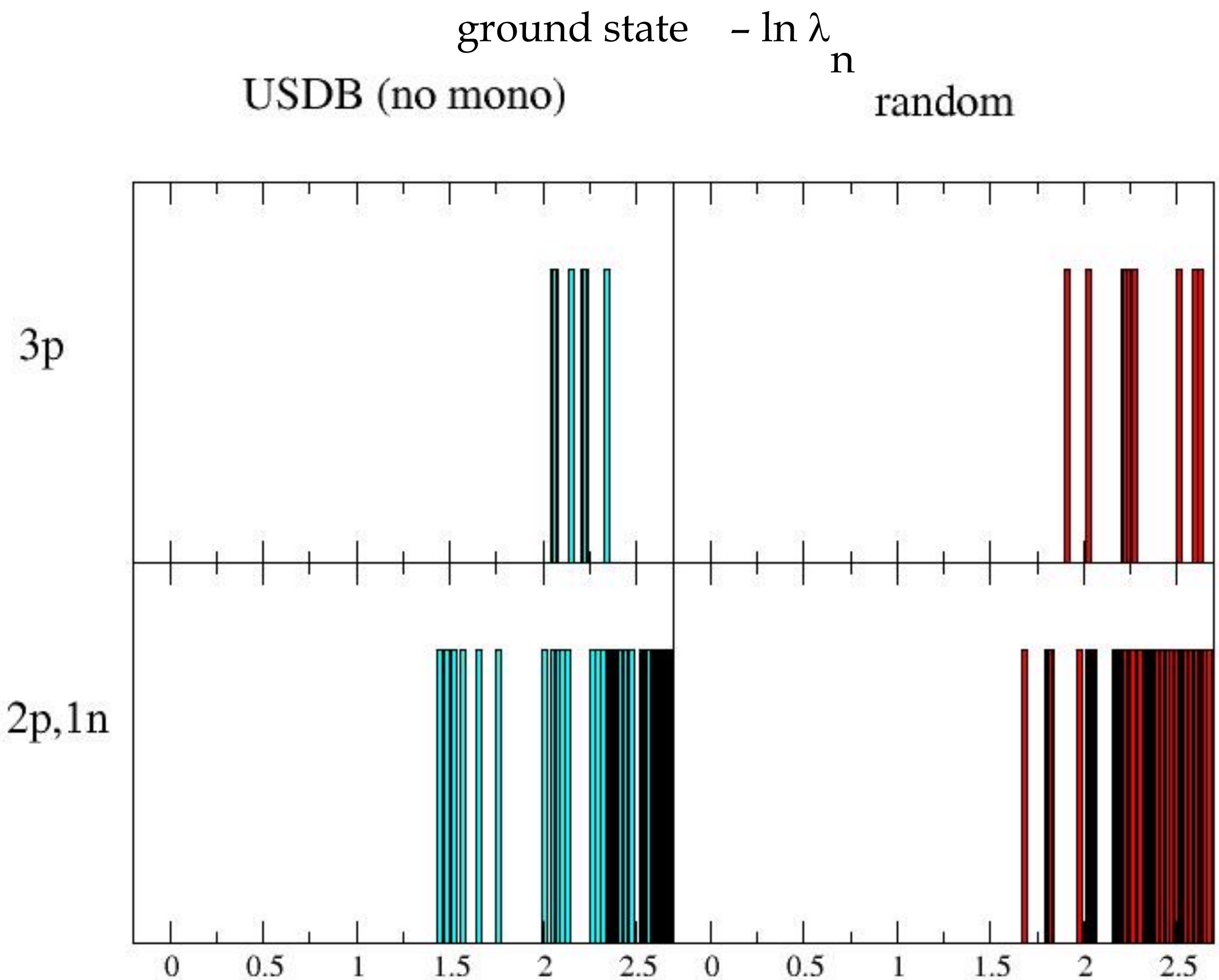
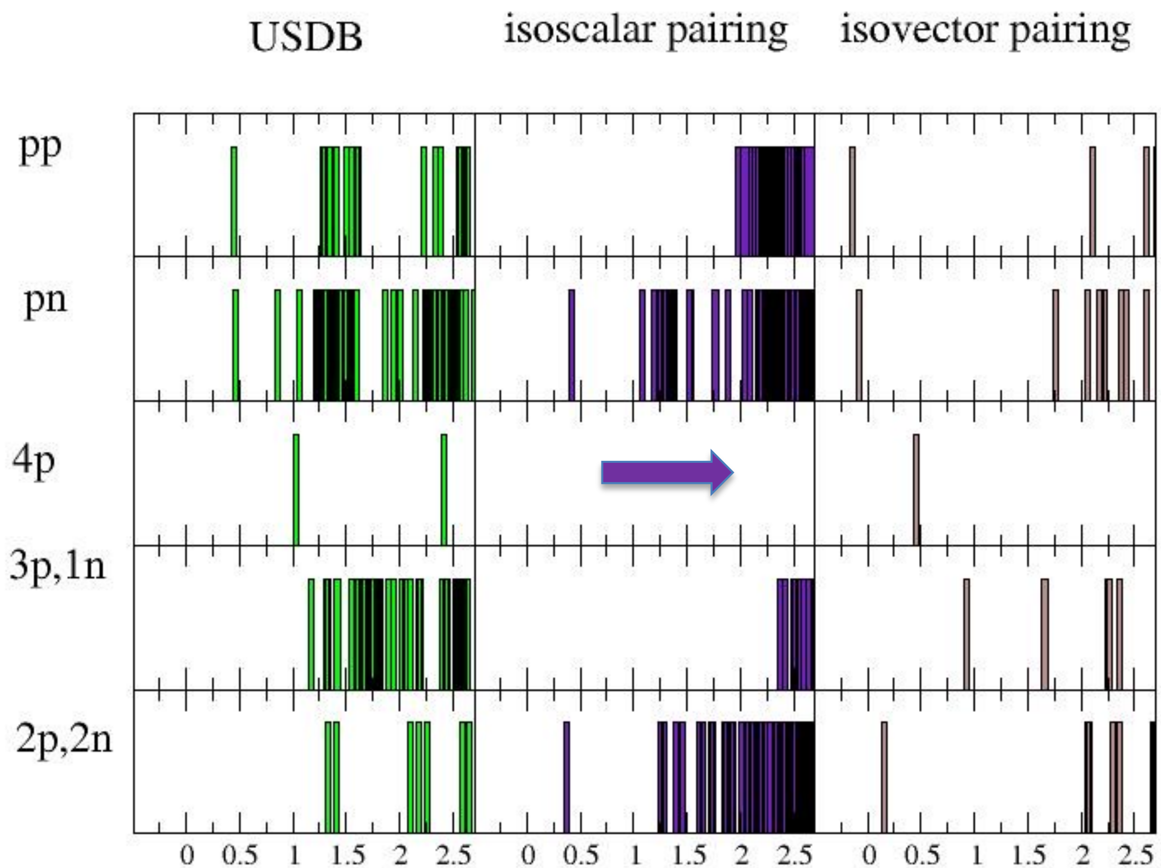



No evidence for strong triplet correlations

# $^{24}$Mg (valence *sd*)

ground state $-\ln \lambda_n$

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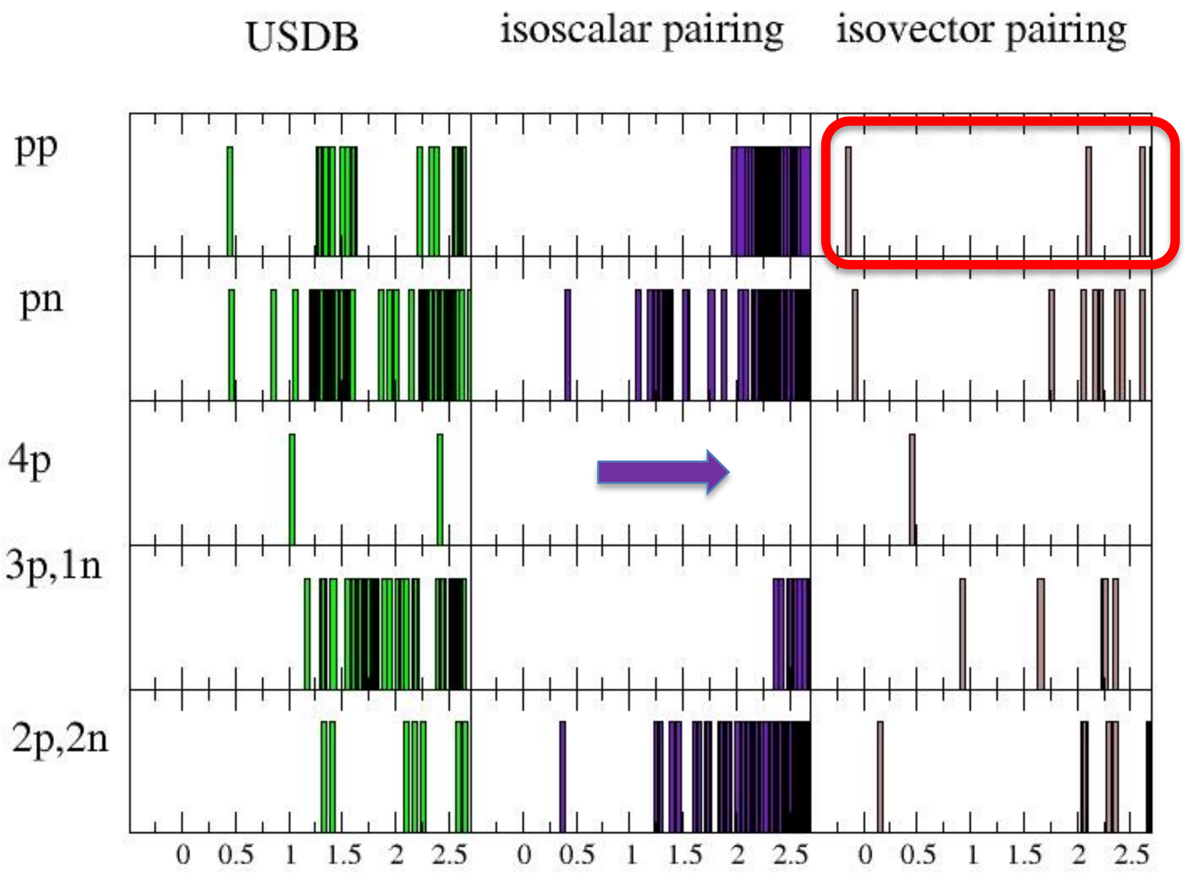

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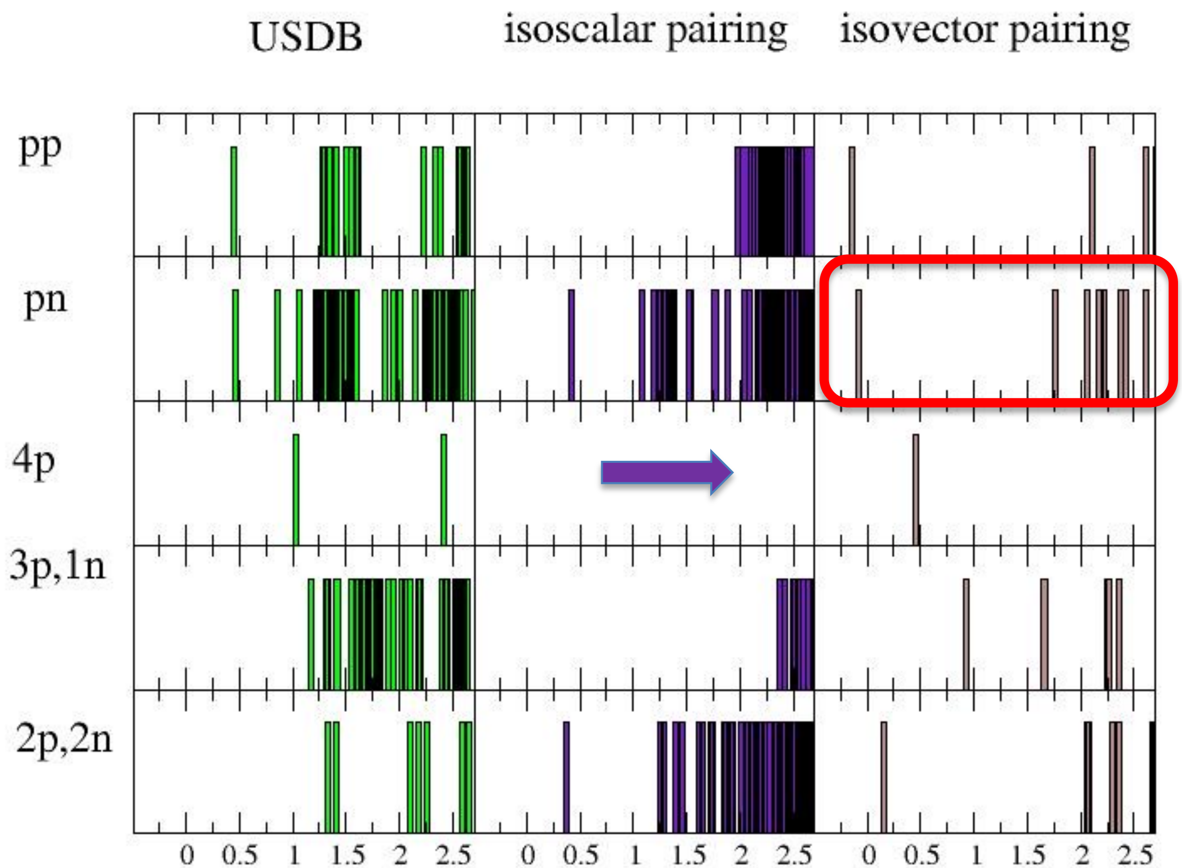

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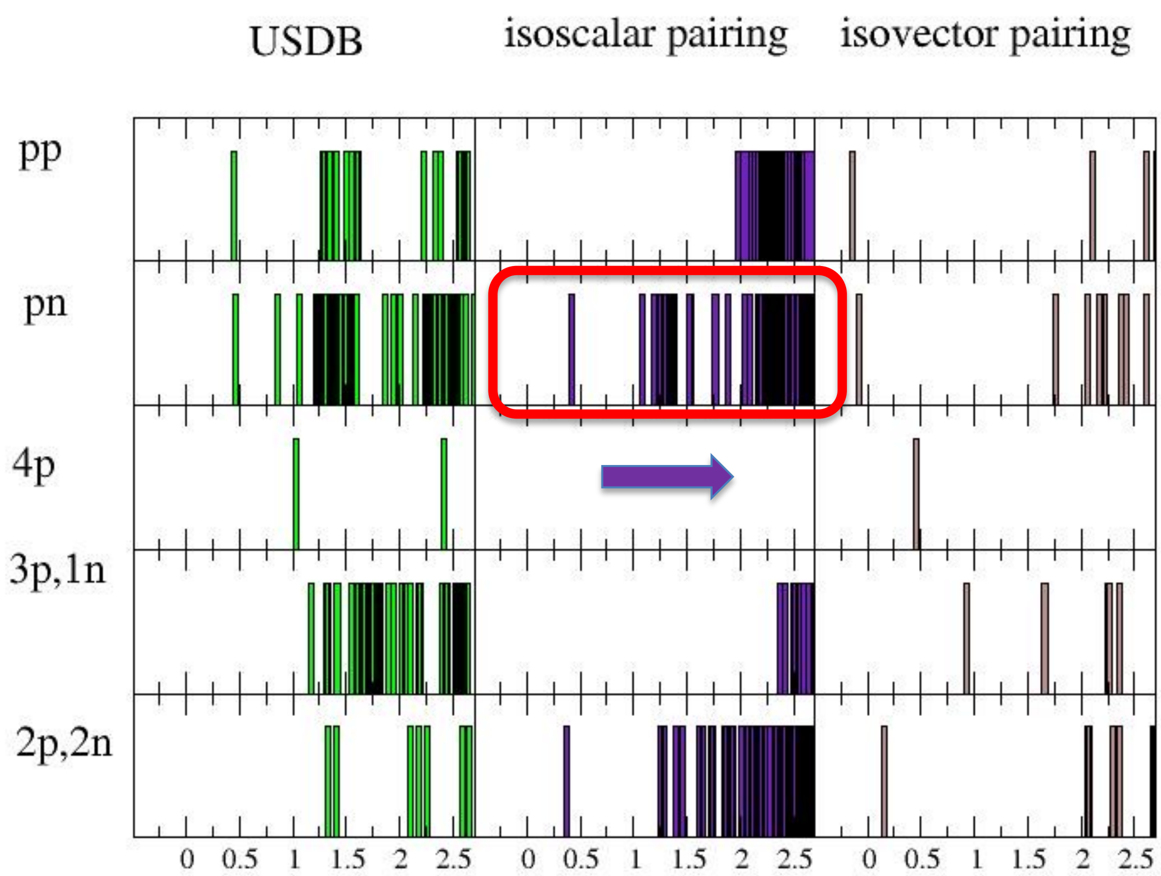

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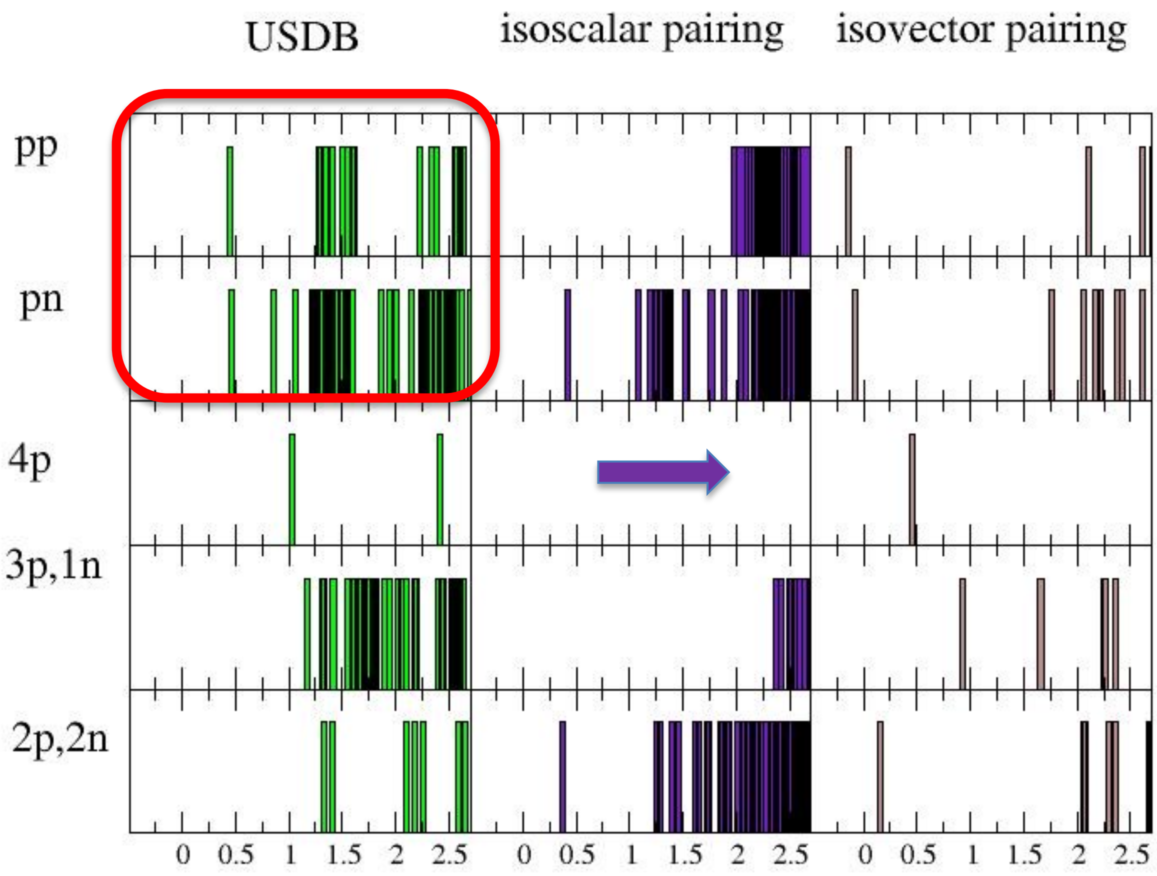

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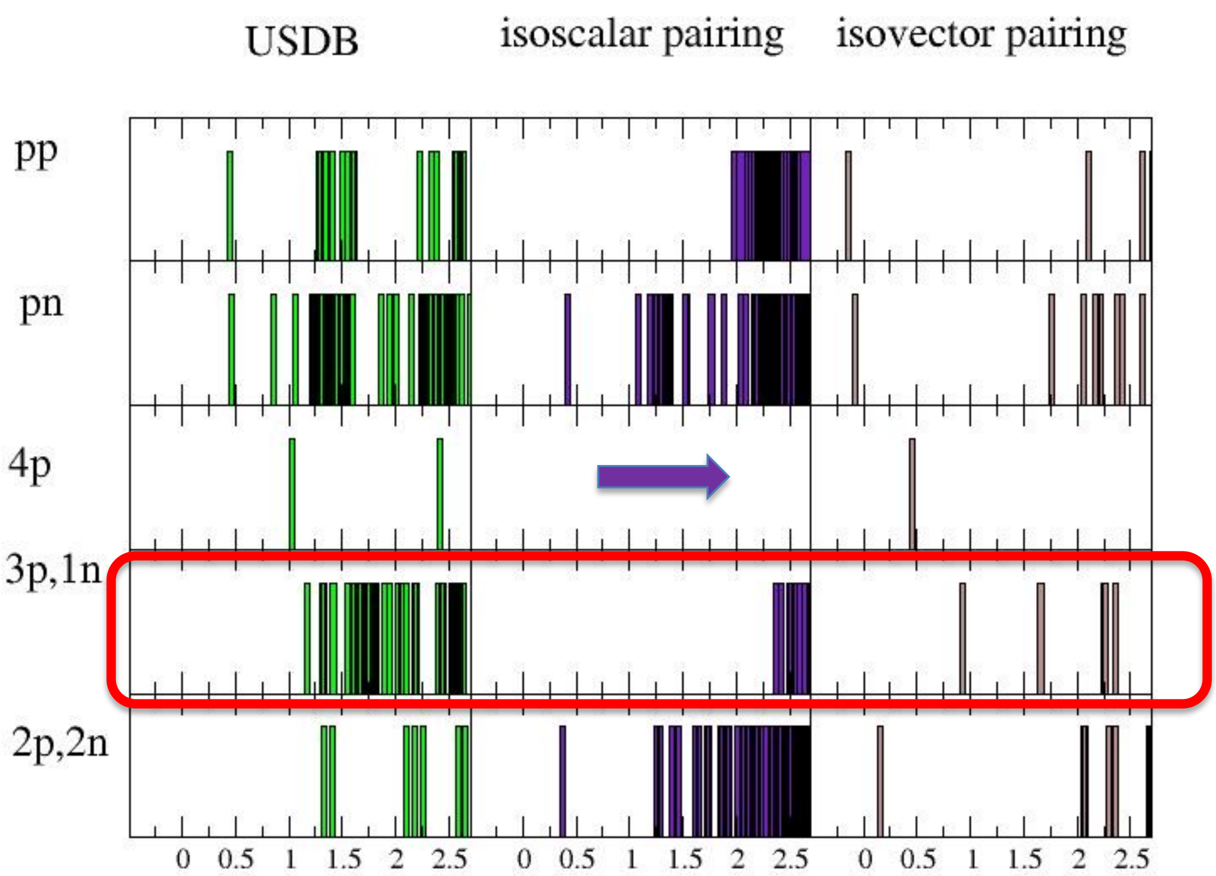


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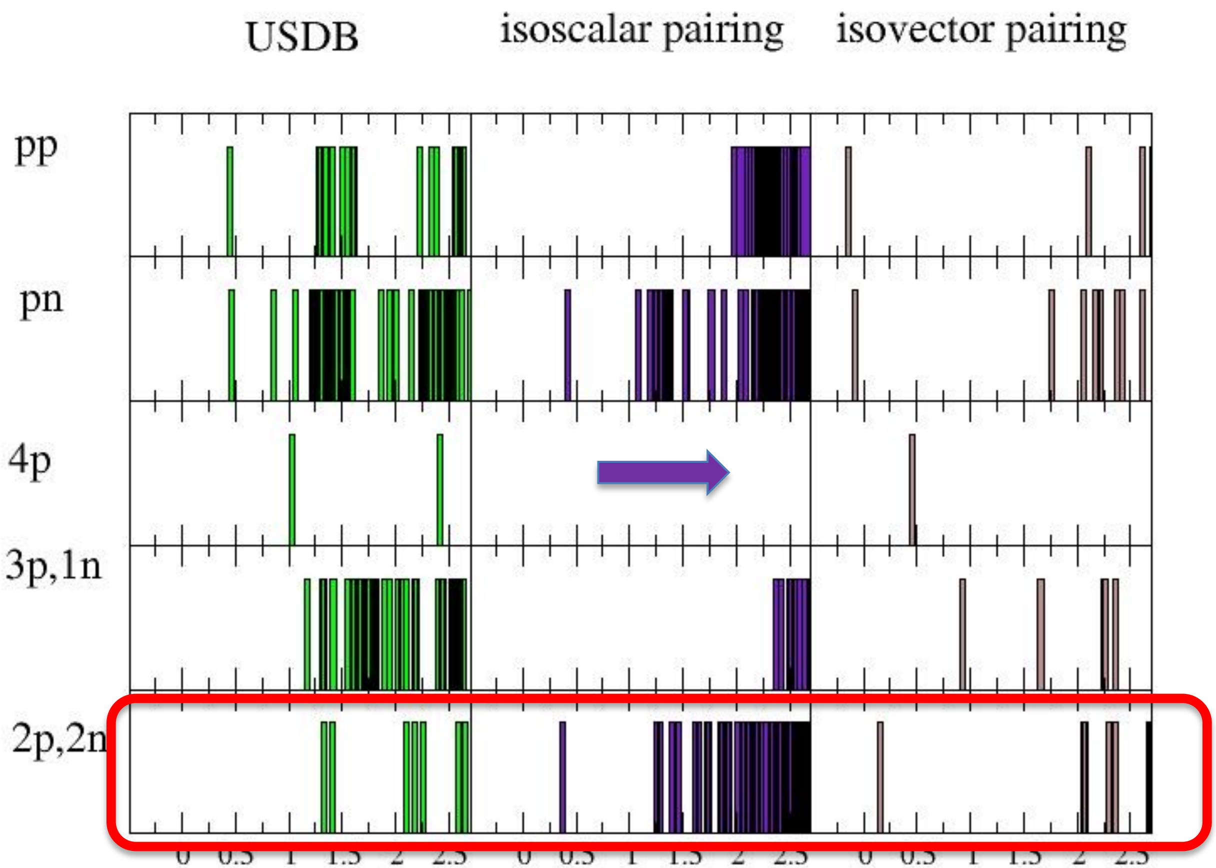
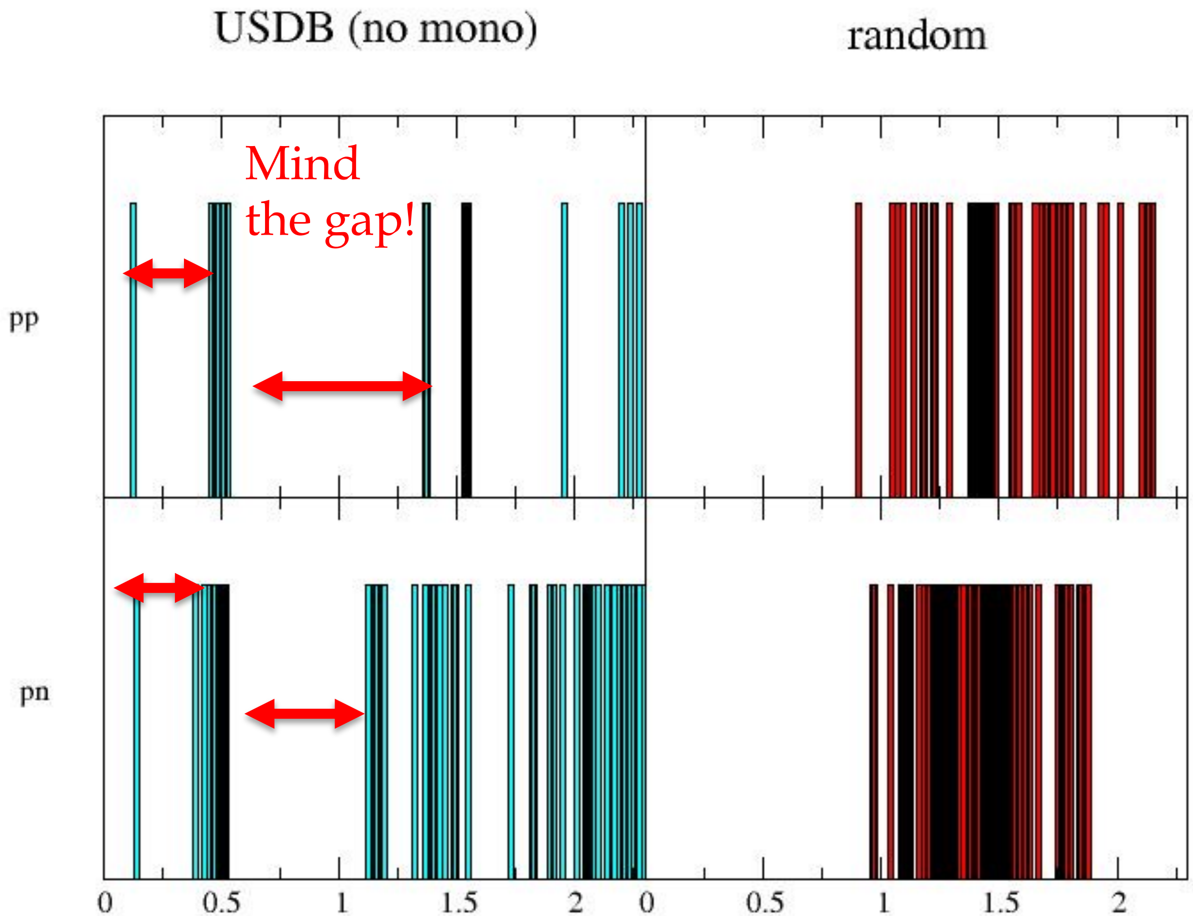
ground state $-\ln \lambda_n$



# $^{28}$ Si (valence *sd*)

ground state $-\ln \lambda_n$

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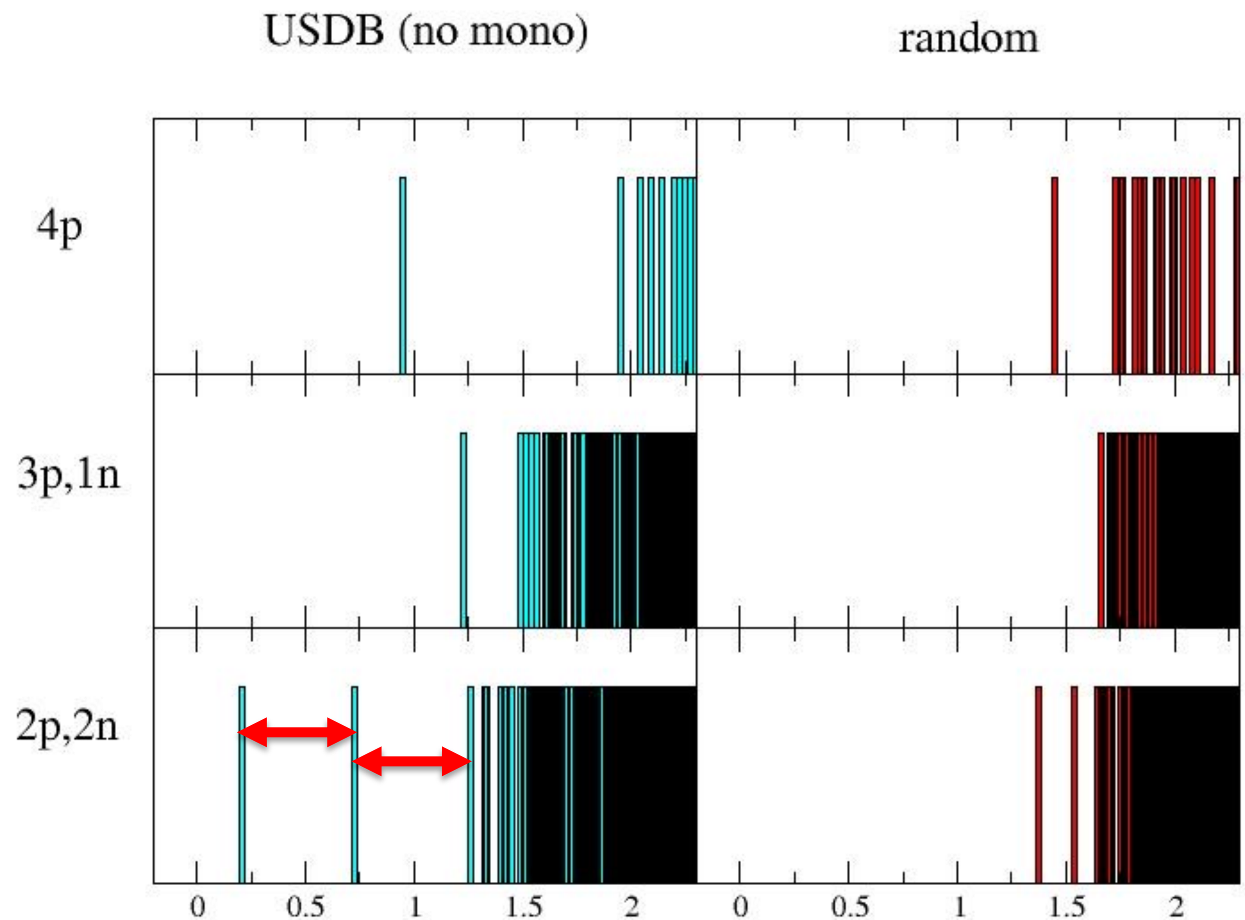
ground state $-\ln \lambda_n$




These have very similar entropies, but some spectra differ

# $^{28}$Mg (valence *sd*)

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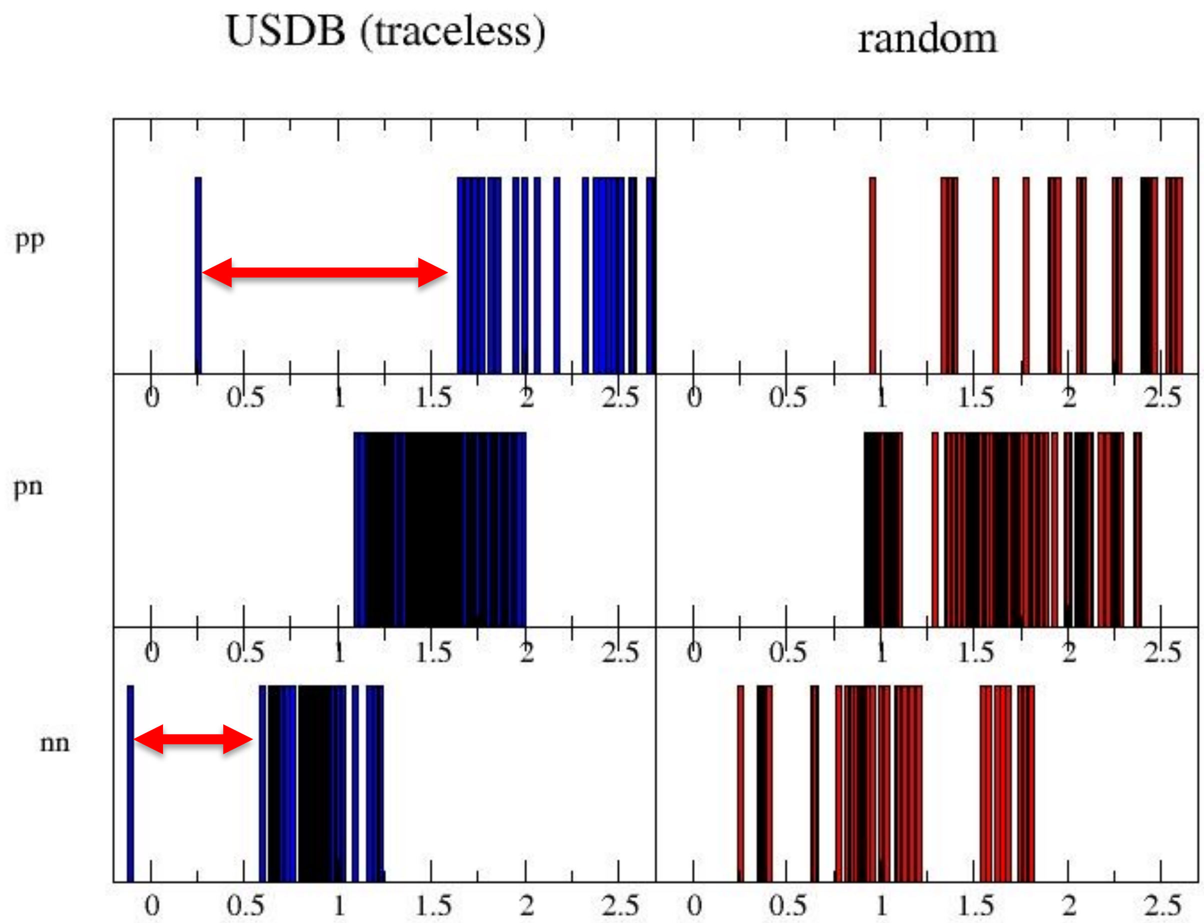
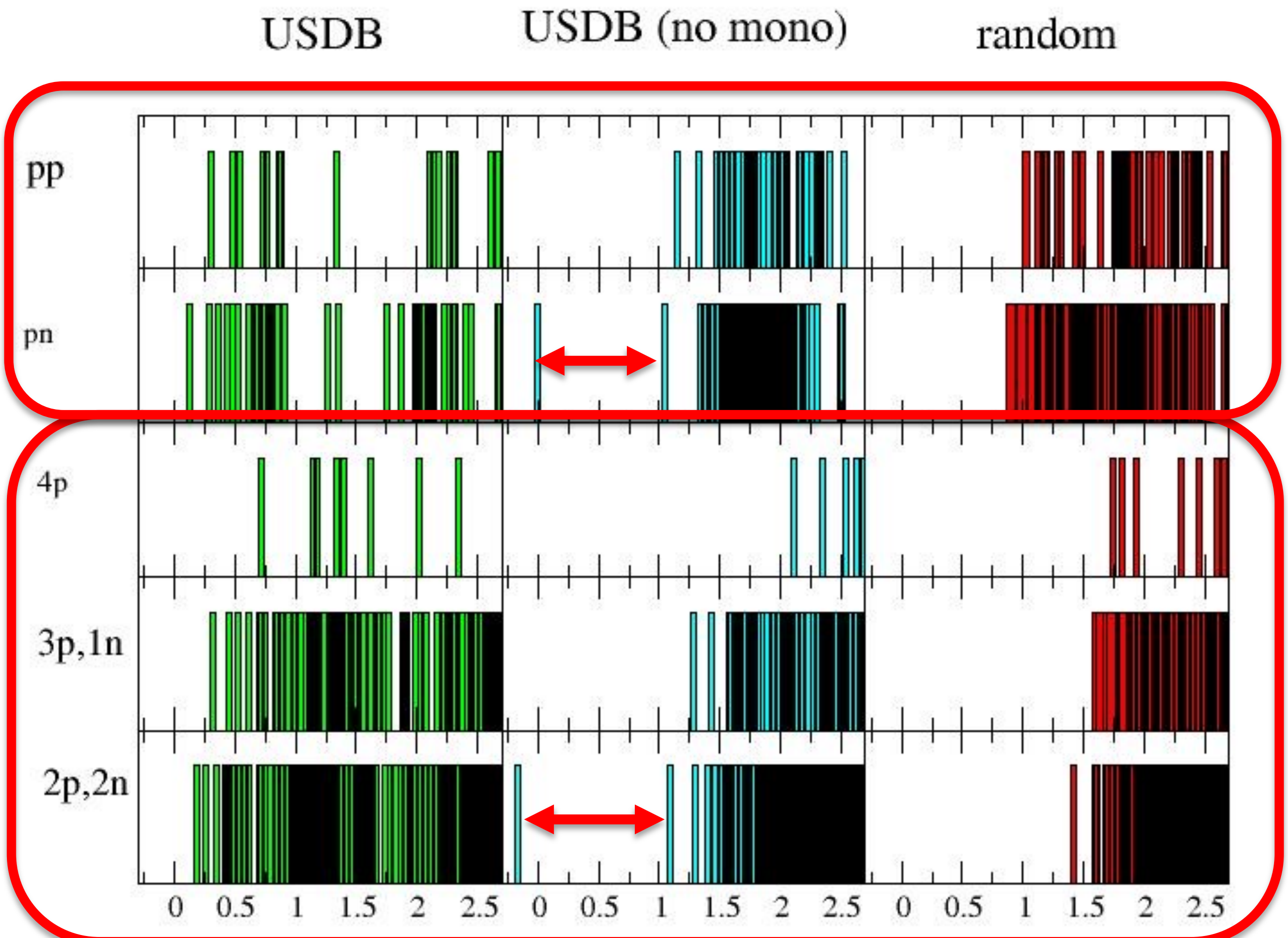


# $^{26}$Al (valence *sd*)

ground state $-\ln \lambda_n$



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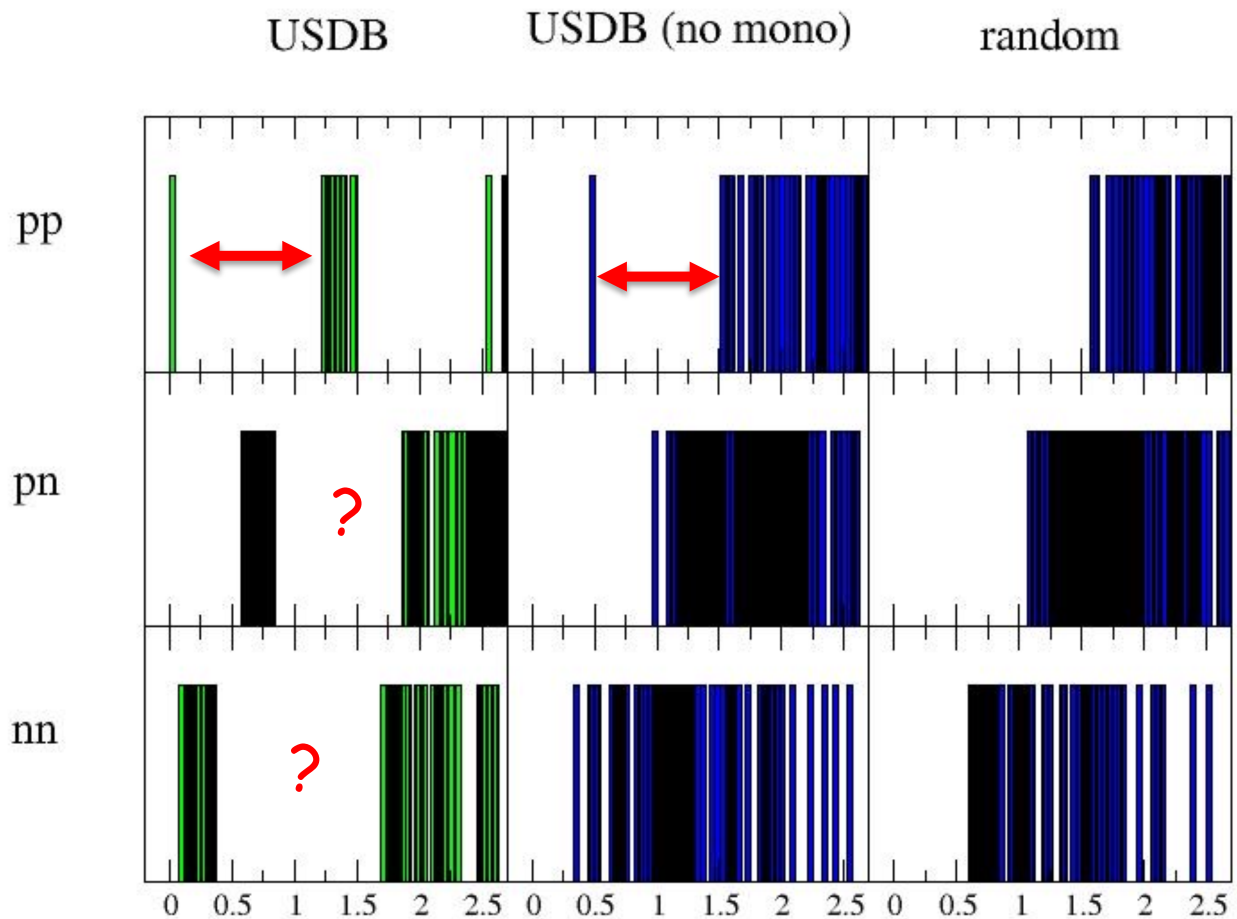
# $^{27}$Mg (valence *sd*)

ground state $-\ln \lambda_n$



# Next steps

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More N > Z, odd-odd, odd-A cases

*fp* shell cases

no-core shell model

Do the trends hold?

(Also: read the literature on entanglement spectra…)

# Another approach

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…which I was going to do on the airplane, before I switched tracks….

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…which I was going to do on the airplane, before I switched tracks….

$$|\Psi^A\rangle = \sum_{i,\alpha} c_{i,\alpha}\, \hat{a}_i^\dagger \otimes |\,\phi_\alpha^{A-a}\rangle$$

A-body state

a-body creation operator

A-a body state

The idea is to treat this as a partitioning into distinguishable sub spaces (which it isn't…)

# Another approach

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$$|\Psi^A\rangle = \sum_{i,\alpha} c_{i,\alpha}\, \hat{a}_i^\dagger \otimes |\,\phi_\alpha^{A-a}\rangle$$

solve

$$\langle\phi_\beta^{A-a}|\hat{a}_j|\Psi^A\rangle = \sum_{i,\alpha} c_{i,\alpha}\langle\phi_\beta^{A-a}|\hat{a}_j\hat{a}_i^\dagger|\phi_\alpha^{A-a}\rangle$$

spectroscopic amplitude

density matrix

# Another approach

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$$| \Psi^A \rangle = \sum_{i,\alpha} c_{i,\alpha} \, \hat{a}_i^\dagger \otimes | \phi_\alpha^{A-a} \rangle$$

solve

$$\langle \phi_\beta^{A-a} | \hat{a}_j | \Psi^A \rangle = \sum_{i,\alpha} c_{i,\alpha} \langle \phi_\beta^{A-a} | \hat{a}_j \hat{a}_i^\dagger | \phi_\alpha^{A-a} \rangle$$

spectroscopic amplitude

density matrix

I *think* this $c_{i,\alpha}$ will be normalized to 1…

# Another approach

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$$|\Psi^A\rangle = \sum_{i,\alpha} c_{i,\alpha}\, \hat{a}_i^\dagger \otimes |\phi_\alpha^{A-a}\rangle$$

Downside: need densities, spectroscopic amplitudes to *all* A-a body states….

solve

$$\langle\phi_\beta^{A-a}|\hat{a}_j|\Psi^A\rangle = \sum_{i,\alpha} c_{i,\alpha}\langle\phi_\beta^{A-a}|\hat{a}_j\hat{a}_i^\dagger|\phi_\alpha^{A-a}\rangle$$

spectroscopic amplitude

density matrix

I *think* this $c_{i,\alpha}$ will be normalized to 1…

**I hope to report on this next workshop!**

# Summary

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The *entanglement spectrum* for a given *a*-body 'cluster', can give clues to which correlations are relevant in many-body systems (especially when contrasted against a 'null case' calculated with a randomly generated interaction).

We clearly see that like-particle pairs and 2 proton, 2 neutron correlations are important, while triplets are not.

The evidence on 1-proton, 1-neutron pairs is less strong.

and finally….

San Diego State University

# Summary

Much work remains to be done!

'ENTANGLEMENT!'