Brown, Sen'kov (MSU)

The CI method applied to valence space calculations in the mass region A=16-60 provide energies and wave functions that can serve as a testing ground for the approximation methods that must be used for UNEDF. An example was provided in the last year by the comparison of Coupled Cluster and CI results for 56Ni. We propose to test extensions of DFT that include correlations such as GCM. This will be done by applying the same Hamiltonian to the CI and deformed approximations.

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[3] **arXiv:0806.3488** [**ps**, **pdf**, **other**]

Many-Body Approximations in the sd-Shell Sandbox

R.A. Sen'kov, G.F. Bertsch, B.A. Brown, Y.L. Luo, V.G. Zelevinsky

Comments: 5 pages, 5 figures

Subjects: **Nuclear Theory (nucl-th)**

A new theoretical approach is presented that combines the Hartree-Fock variational scheme with the exact solution of the pairing problem in the finite orbital space. Using this formulation in the sd-space as an example, we show that the exact pairing significantly improves the results for the ground state energy

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As in most mean-field approaches, we formulate this method as variational one. As in the shell model, we assume a general form of the two-body Hamiltonian that includes the single-particle term t and the (antisymmetrized) two-body interaction V:

$$\hat{H} = \sum_{ik} t_{ik}\, a_i^\dagger a_k + \frac{1}{4} \sum_{ijkl} V_{ijkl}\, a_i^\dagger a_j^\dagger a_k a_l. \qquad (1)$$

The variational wave function $|\Psi\rangle$ will be defined below. The wave function and all properties of the system follow from the minimization of the expectation value

$$\langle \Psi | \hat{H} | \Psi \rangle. \qquad (2)$$

The ground state wave function $|\Psi\rangle$ for a fixed particle number N can be presented as a superposition of basis states,

$$|\Psi\rangle = \sum_{d \in D} C_d |d\rangle, \qquad (3)$$

where each basis state $|d\rangle$ is a Slater determinant which for N fermions can be written as usual:

$$|d\rangle = a_{\nu_1}^\dagger a_{\nu_2}^\dagger \ldots a_{\nu_N}^\dagger |0\rangle. \qquad (4)$$

Exact pairing in a spherical basis

$$\prod_{j;m>0} a^{\dagger}_{jm} a^{\dagger}_{j\tilde{m}} |0\rangle, \qquad (5)$$

[4] A. Volya, B.A. Brown, and V. Zelevinsky, Phys. Lett. B **509**, 37 (2001).

[5] V. Zelevinsky and A. Volya, Phys. Atom. Nucl. **66**, 1829 (2003).

Using SU(2) quasi-spin algebra

For example for 5 orbits (tin isotopes) the matrix dimension is at most 2000

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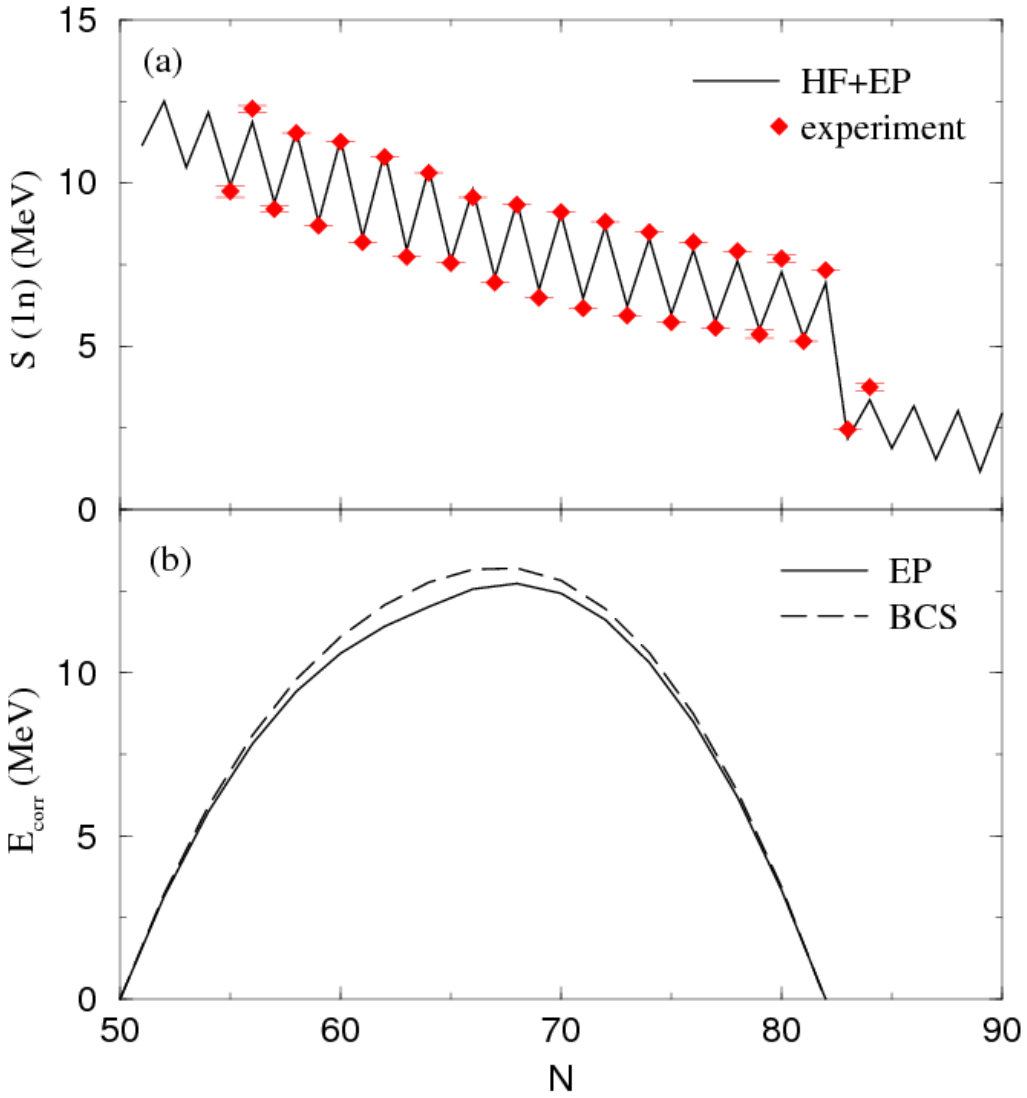
Sn isotopes Skx +EP (renormalized G matrix)



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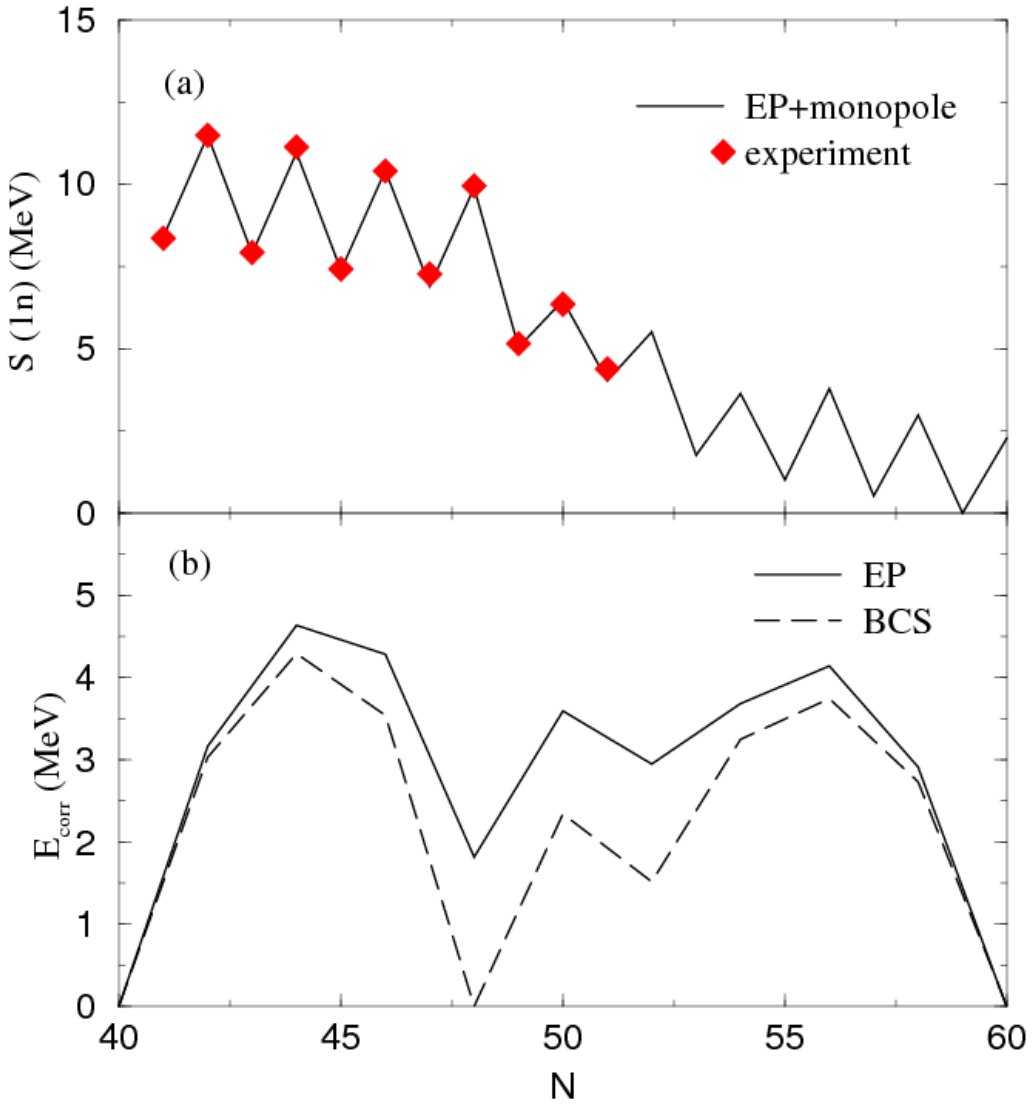
Ca isotopes Skx +EP (renormalized G matrix)



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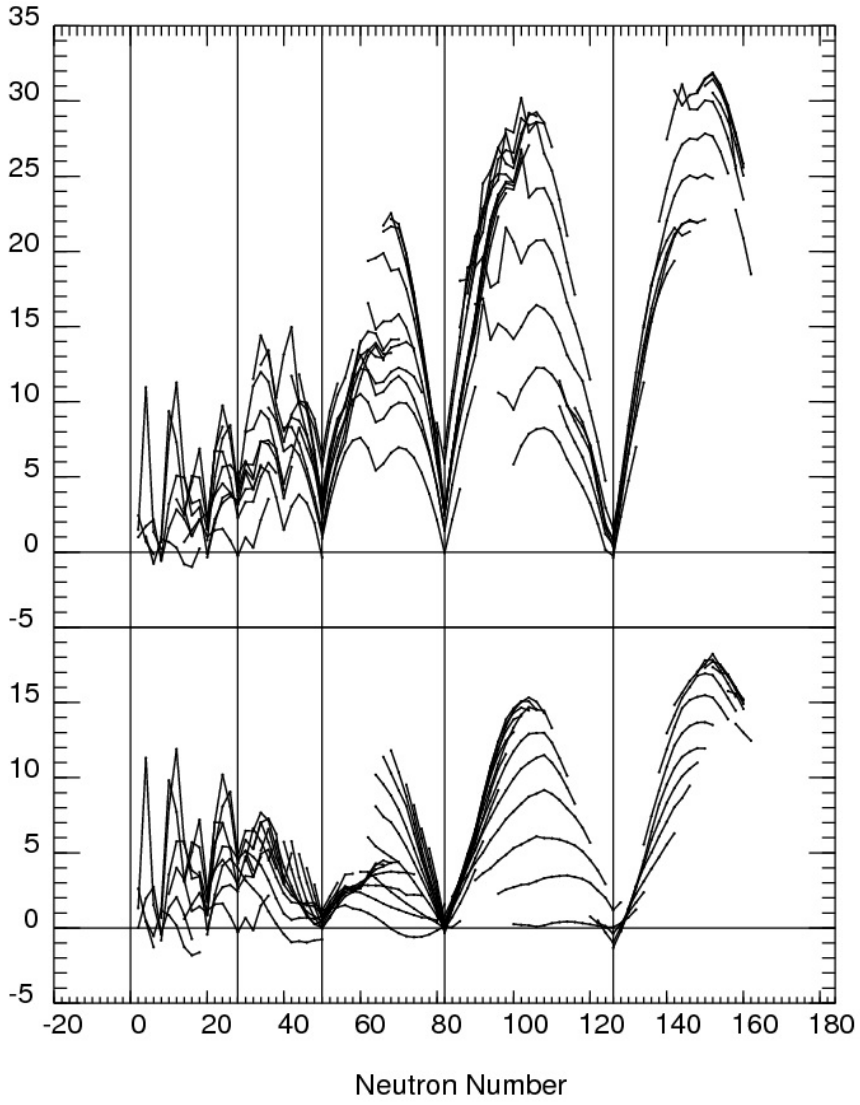
Spherical basis calculations with Skx – 2001
BE(exp) – BE(theory)



DFT (Skx)

DFT(Skx) + exact pairing
(renormalized G matrix)

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Exact pairing in a deformed basis

According to the Kramers theorem, the orbitals $|\nu m\rangle$ and $|\nu - m\rangle$ are degenerate. However, the pairs may also be formed by the states m and $-m$ belonging to different sets of remaining quantum numbers. Thus, for our basis Slater determinants $|d\rangle$ we assume the following form:

$$\prod_{\nu,\kappa;m>0} a^{\dagger}_{\nu m} a^{\dagger}_{\kappa -m} |0\rangle . \qquad (6)$$

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The variation over amplitudes C_d with the additional normalization condition of the wave function, $\langle\Psi|\Psi\rangle = 1$, leads us to the usual set of equations,

$$\sum_{d'}\langle d|\hat{H}|d'\rangle C_{d'} = EC_d. \tag{7}$$

The matrix elements $\langle d|\hat{H}|d'\rangle$ are calculated for the determinants built on a given single-particle basis, and equations (7) are solved numerically. The mean-field basis is found from the self-consistent HF equations:

$$h(\rho)\phi_\nu = \epsilon_\nu\phi_\nu, \tag{8}$$

where

$$h(\rho) = t + V(\rho) \tag{9}$$

$$\rho_{ij} = \langle\Psi|a_j^\dagger a_i|\Psi\rangle. \tag{10}$$

The mean field potential is given by its matrix elements,

$$V_{ij}(\rho) = \sum_{kl} V_{iklj}\rho_{lk}. \tag{11}$$

The HFP scheme of solution is the following:

- Start with the spherical single-particle basis $|\kappa m\rangle$
- Choose in this basis the initial diagonal density matrix ρ corresponding to occupation numbers specific for prolate or oblate shapes (pairs with small or large $|m|$, respectively)
- Solve the HF variational equation (8) and get the single-particle spectrum (ϕ_ν, ϵ_ν), in general corresponding to a deformed field
- Construct the "paired" class of many-body basis wave functions according to eq. (6) and calculate the matrix elements of the Hamiltonian H
- Solve the variational equation (7) and obtain the ground state wave function
- Calculate the next-step density matrix (10)
- Repeat the procedure starting from the step three until convergence

$$E_{\mathrm{HFP}} = \langle \Psi | \hat{H} | \Psi \rangle. \qquad (12)$$

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For our test of the methods, we will take for V the USDB interaction from the *sd*-shell model [6]. It will allow us to compare the results obtained using our approximate method with the exact shell model calculations in the same single-particle model space.

[6] B.A. Brown and W.A. Richter, Phys. Rev. C **74**, 034315 (2006).

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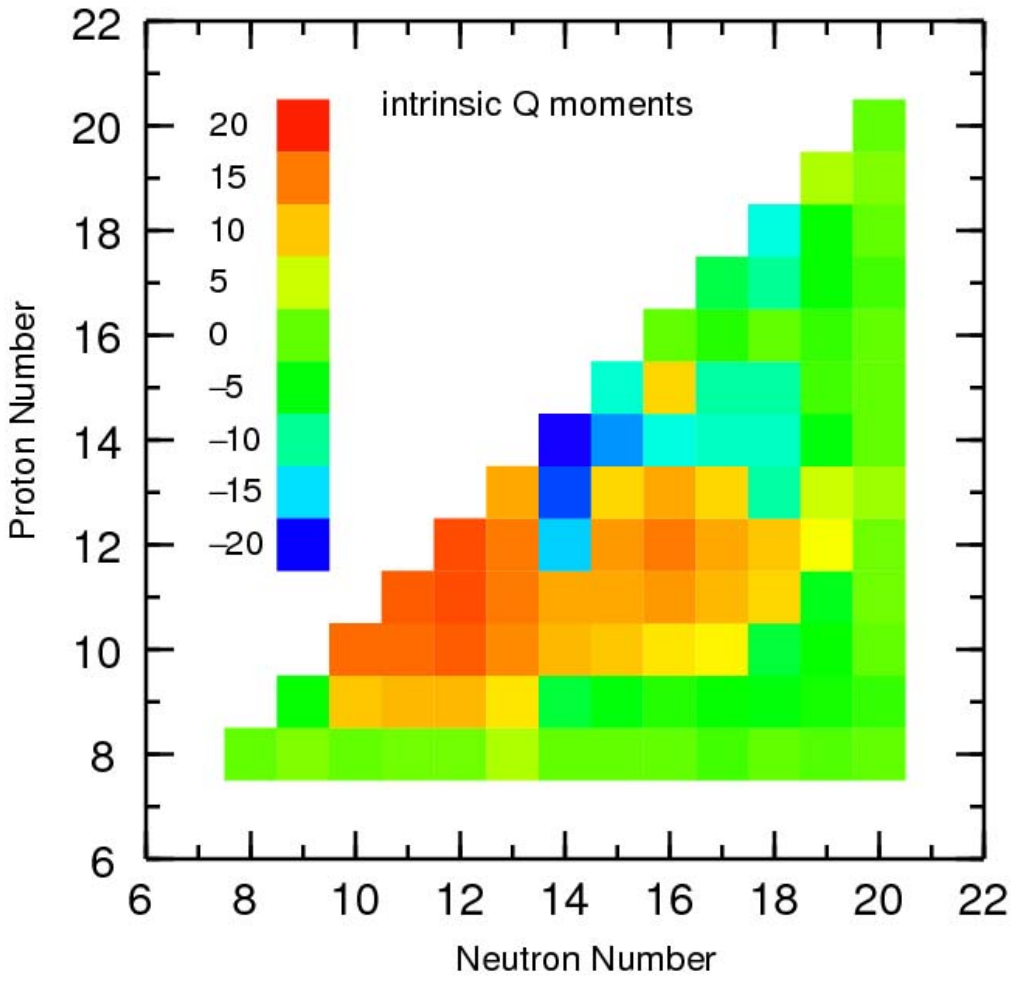
In many cases there are two minima and the lowest energy must be found from several starting densities.
Intrinsic Q moments of the lowest energy state (in units of b^2)



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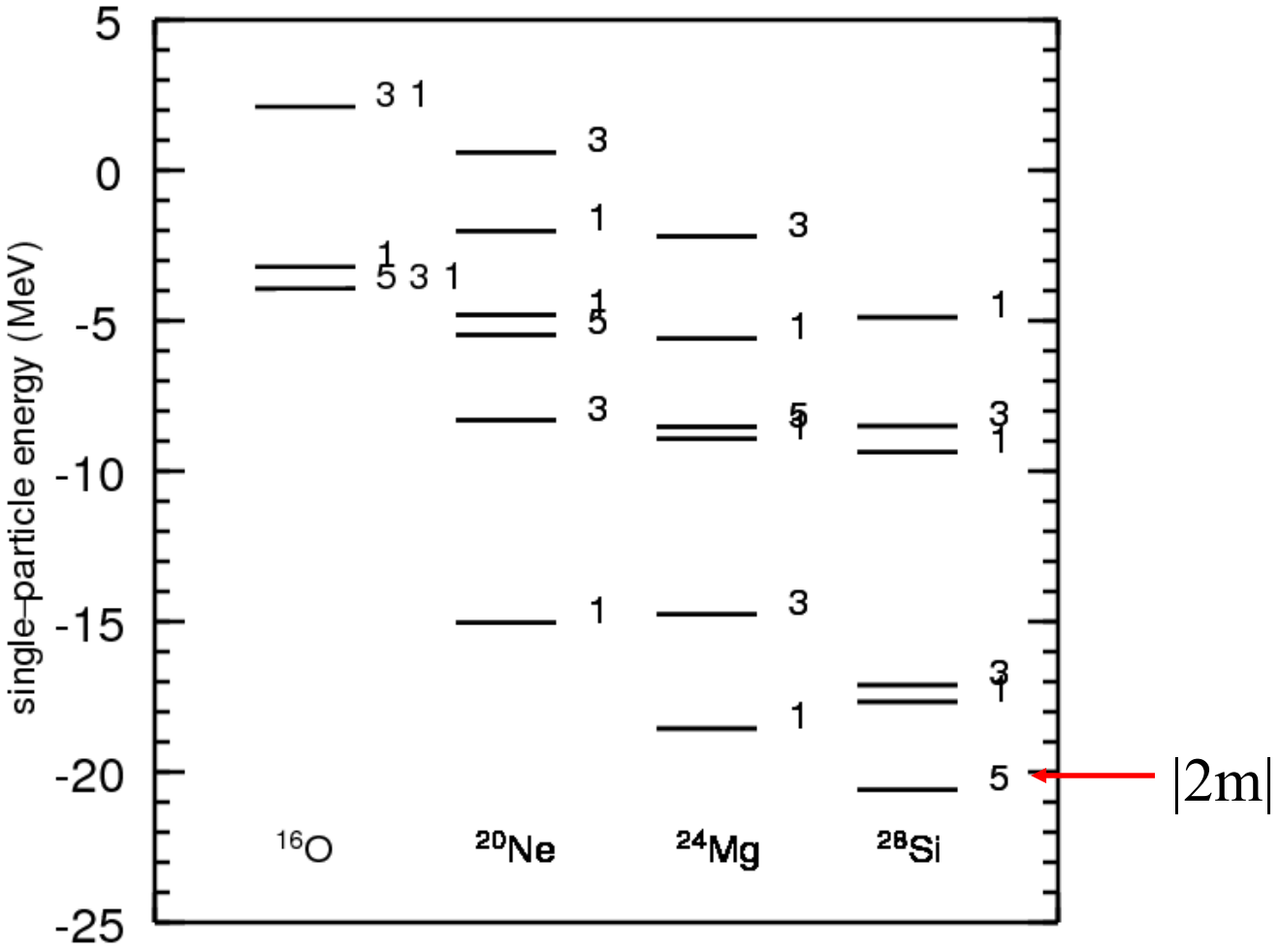
$\varepsilon(|m|)$



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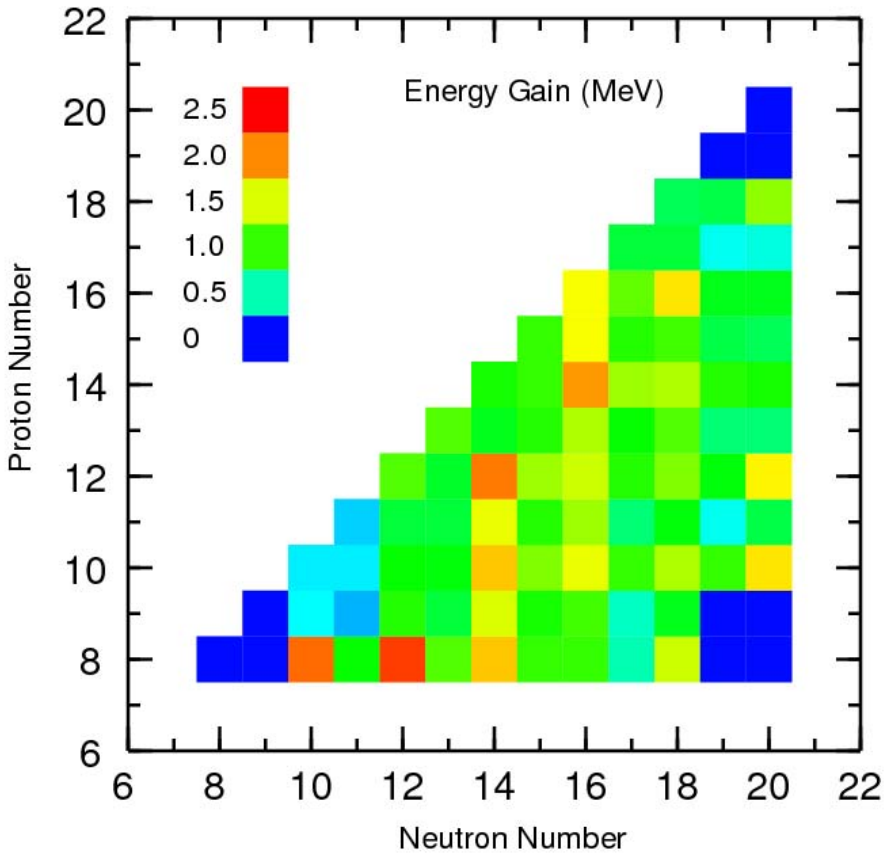
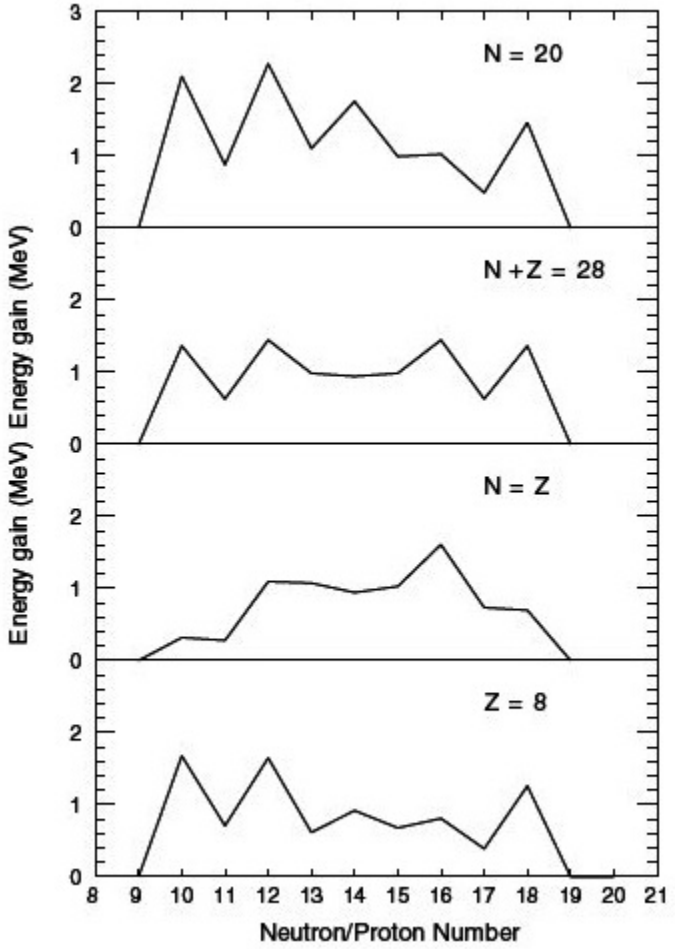
$$E_{\mathrm{corr}} = E_{\mathrm{HF}} - E_{\mathrm{HFP}}. \qquad (13)$$





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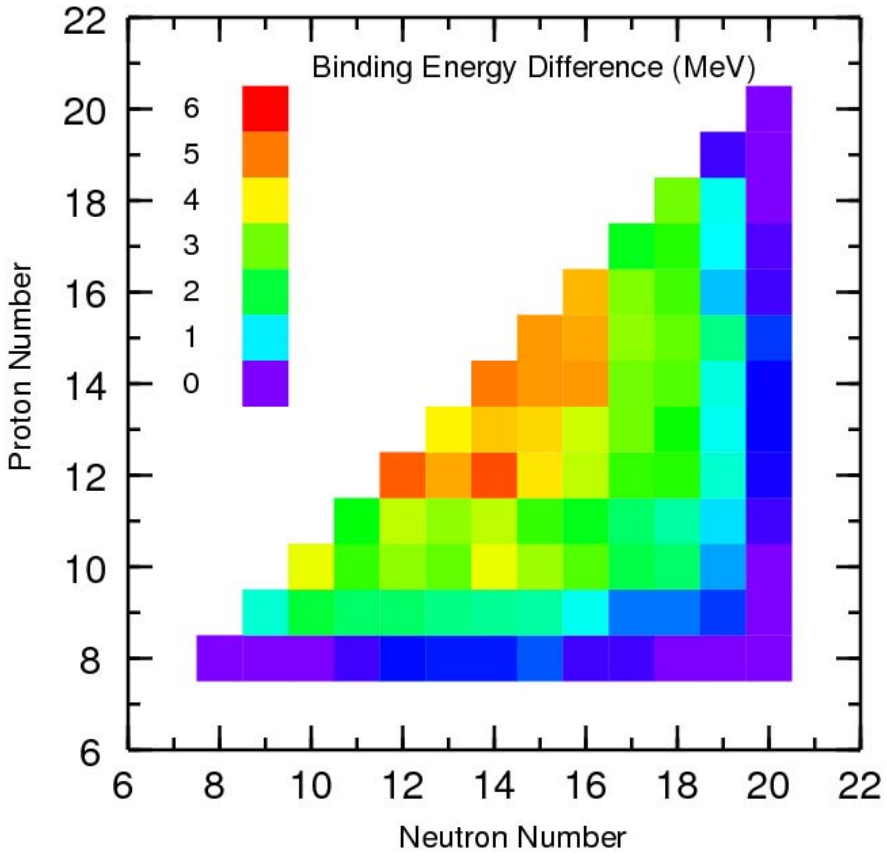
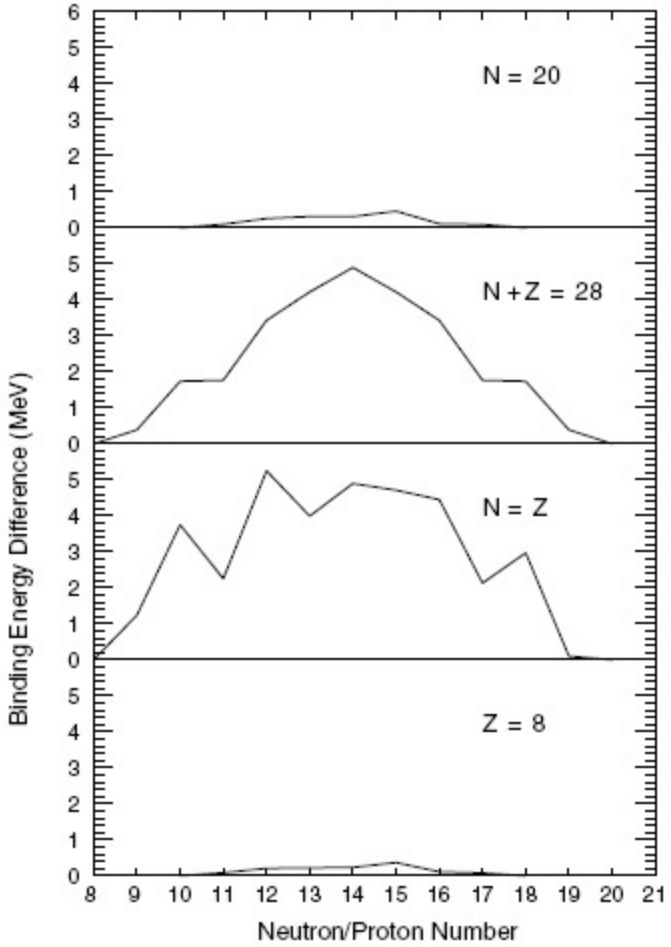
Full sd compared to HFP





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What's next

Still have up to 5 MeV to go to agree with exact sd results

PN pairing (J=0 T=1 and J=1 T=0 and alpha cluster)

Angular-momentum projection

Non-axial symmetry

Application to pf and higher shells

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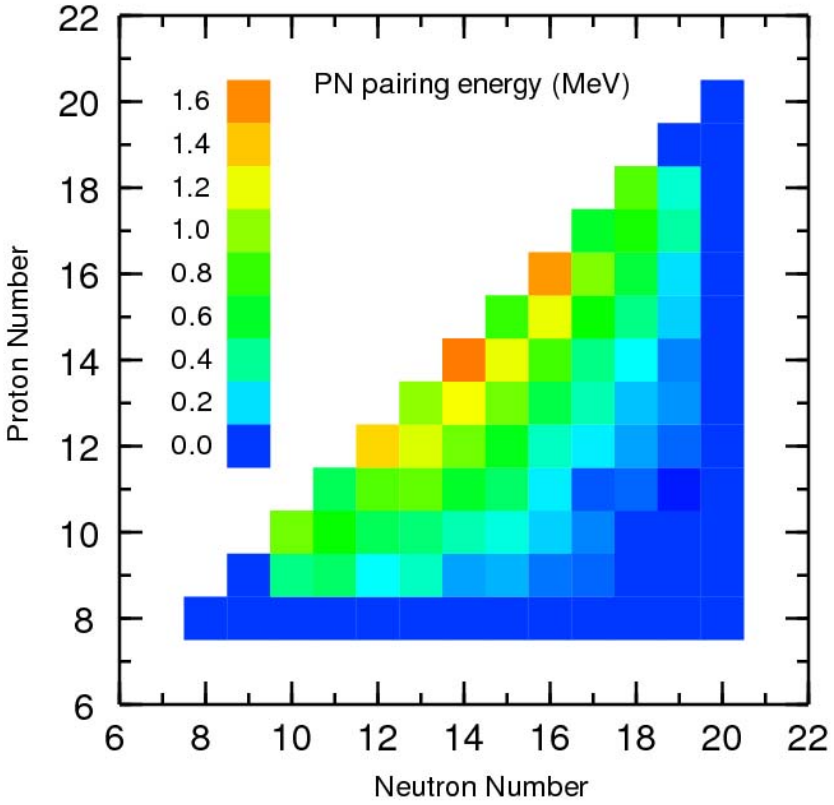
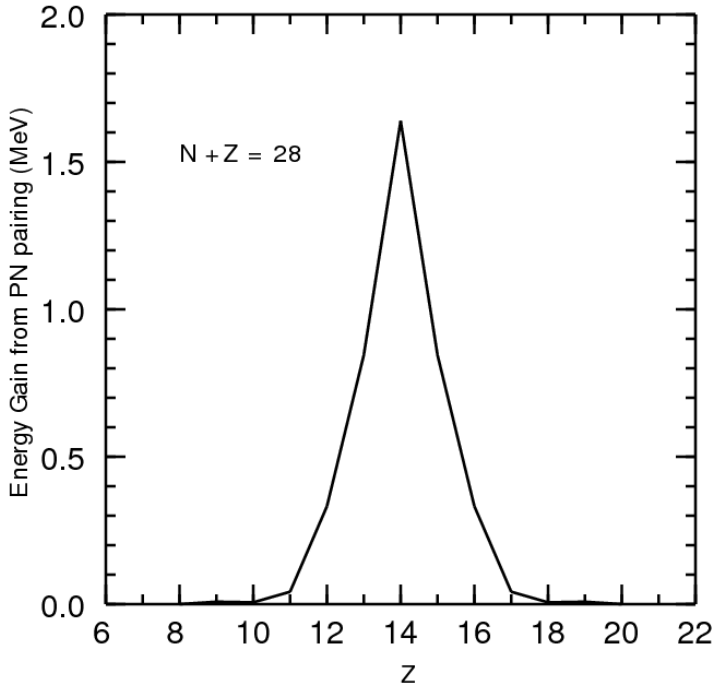
Full sd with and without the off-diagonal PN (J=0, T=1) tbme





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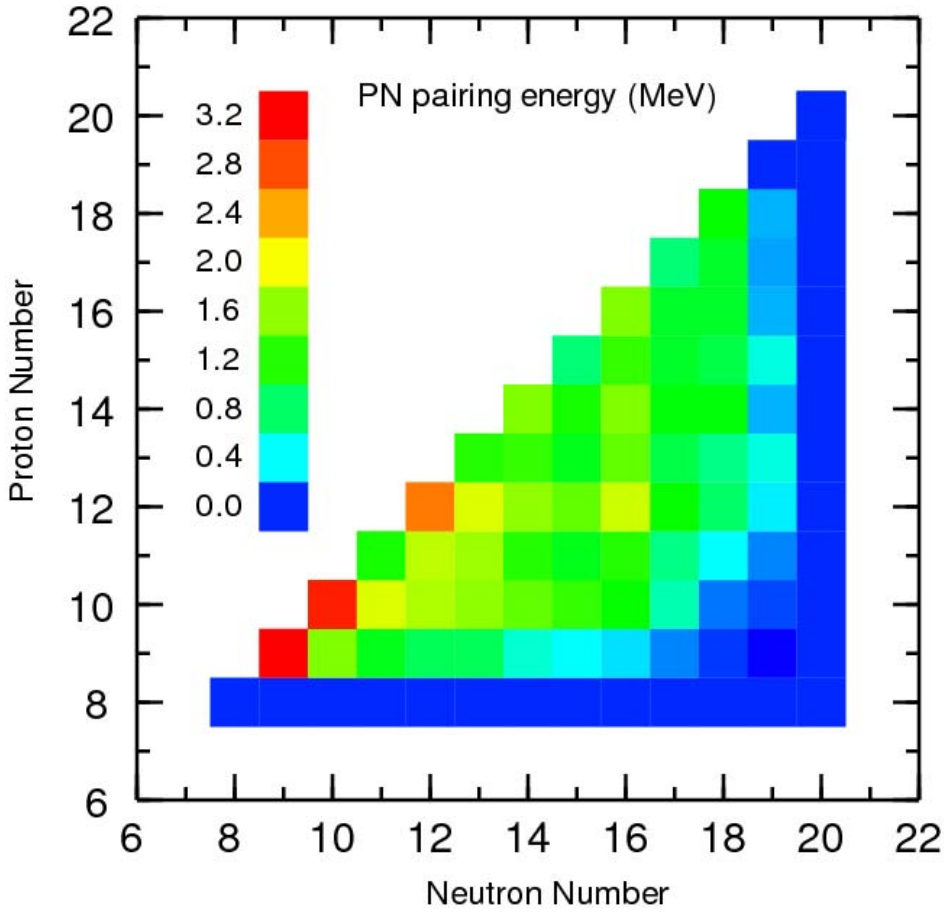
Implemention of PN (J=0, T=1) pairing

For T=0, T=1/2 isospin symmetry means that PP=NN=PN e.g. adding PN means just mutiplying NN+PP by 1.5

For higher T it drops off fast and might be approximated (or ignored)

Full sd with and without the off-diagonal PN (J=1, T=0) tbme important also for odd-odd nuclei
(already in the deformed part?)



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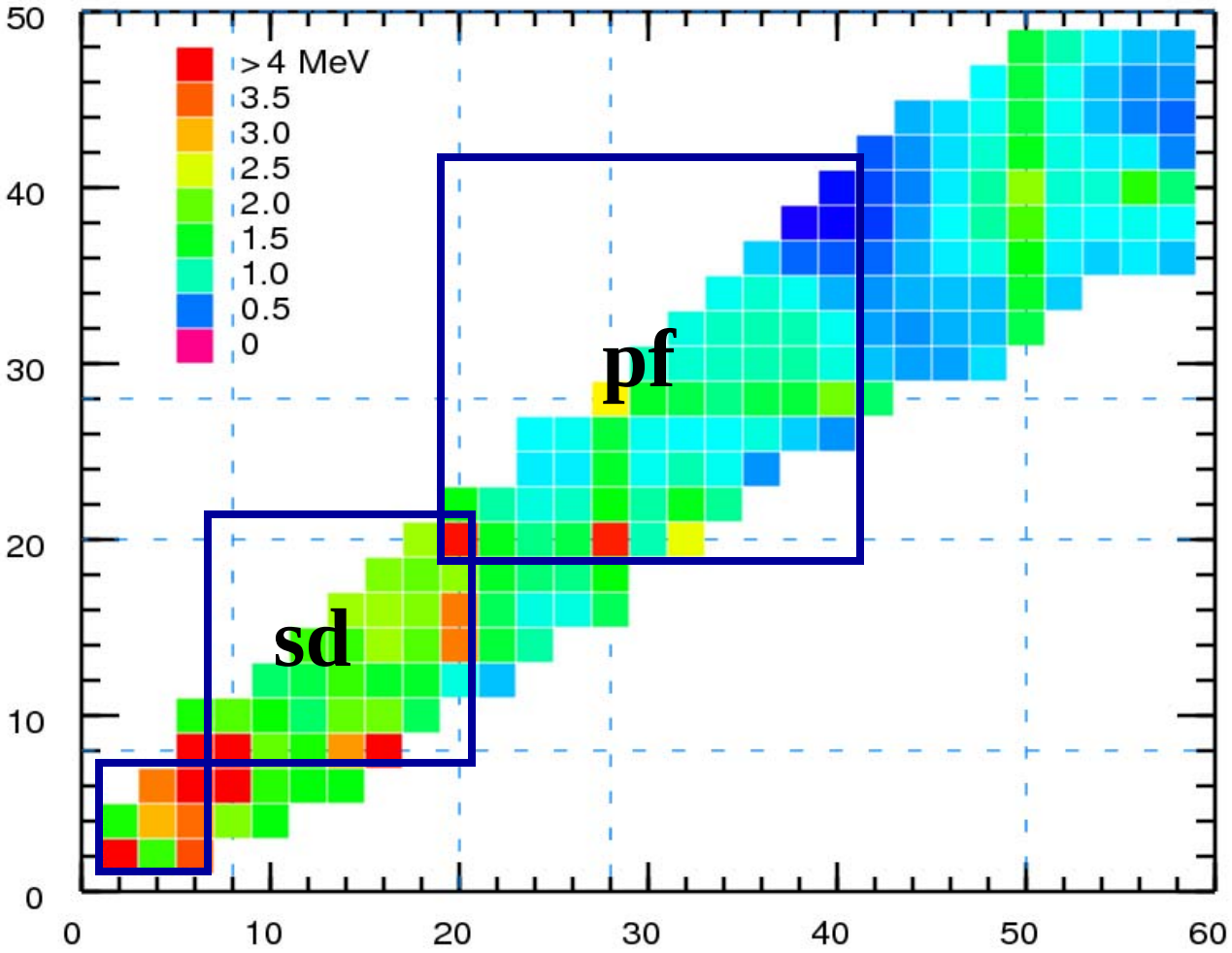

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DFT ←→ CI

HFP and PCI provides a new tool for CI in very large model spaces
- use as first test of effective Hamiltonians

HFP provides a way to improve the pairing part of DFT particularly in the region up to A=100

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1. What are the main accomplishments since the last meeting? Is your Year-2 plan well on track? If not, why? Project completed and paper done.

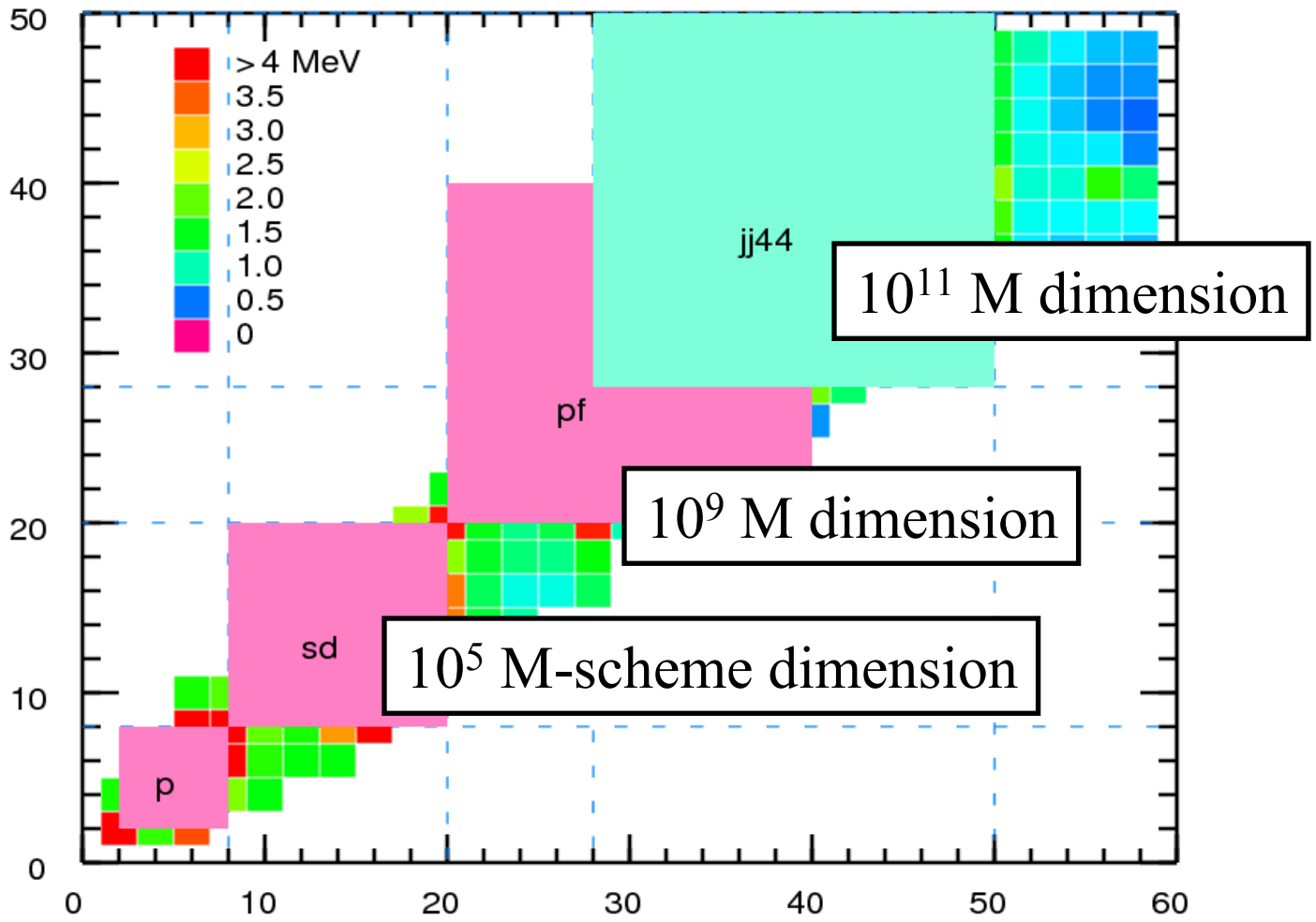
2. What are the aspects of your science that require high- performance computing?
None in UNEDF
OR What problems in high performance computing are you working on in general?
NuShellx for CI

3. What are the major computational issues? Are there any questions you would like to bring to the attention of our CS/AM collaborators? OR Are there general capabilities of your computer science work that might be of interest to other physicists than the ones you are currently working with?
NuShellx with openMP

4. What is the detailed roadmap of your project for the remaning part of Year-2 and Year-3? Could you sketch the workplan for Years 4 and 5?
Apply HFP to fp and higher shells.
Think about J projection and other improvements to HFP

5. Are there any "showcase" (i.e., of Nature/Science caliber) physics and computational questions that you are hoping to answer in Years 2 and 3? (outside of UNEDF)
First CI calculations for A=56-100 region - crucial for astrophysics, weak interaction physics and nuclear structure

The CI computational challenge



jj44 means $f_{5/2}$, $p_{3/2}$, $p_{1/2}$, $g_{9/2}$ orbits for protons and neutrons

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NuShellx – Bill Rae - 2008

- Like the NATHAN code but faster (10 times?) and open-source
- NuShellx@MSU is a user friendly wrap with standard input and output
- H matrix elements calculated "on-the-fly" – no matrix to store
- All a+, a+a, and a+a+ matrix elements can be calculated as well as overlaps for any two-body operator
- Basis in Jp Jn can be truncated – and particle-hole (proton-neutron) interaction can be diagonalized to keep only the most collective components
- OpenMP used with high efficiency – tested up to 32 cores should go up to about 100 cores
- Each J and each nucleus can be spread over nodes – so in principle 1000 nodes x 8 cores or more could be used efficiently
- Many levels for a given J much easier than in M-scheme (coexisting shapes – level density)

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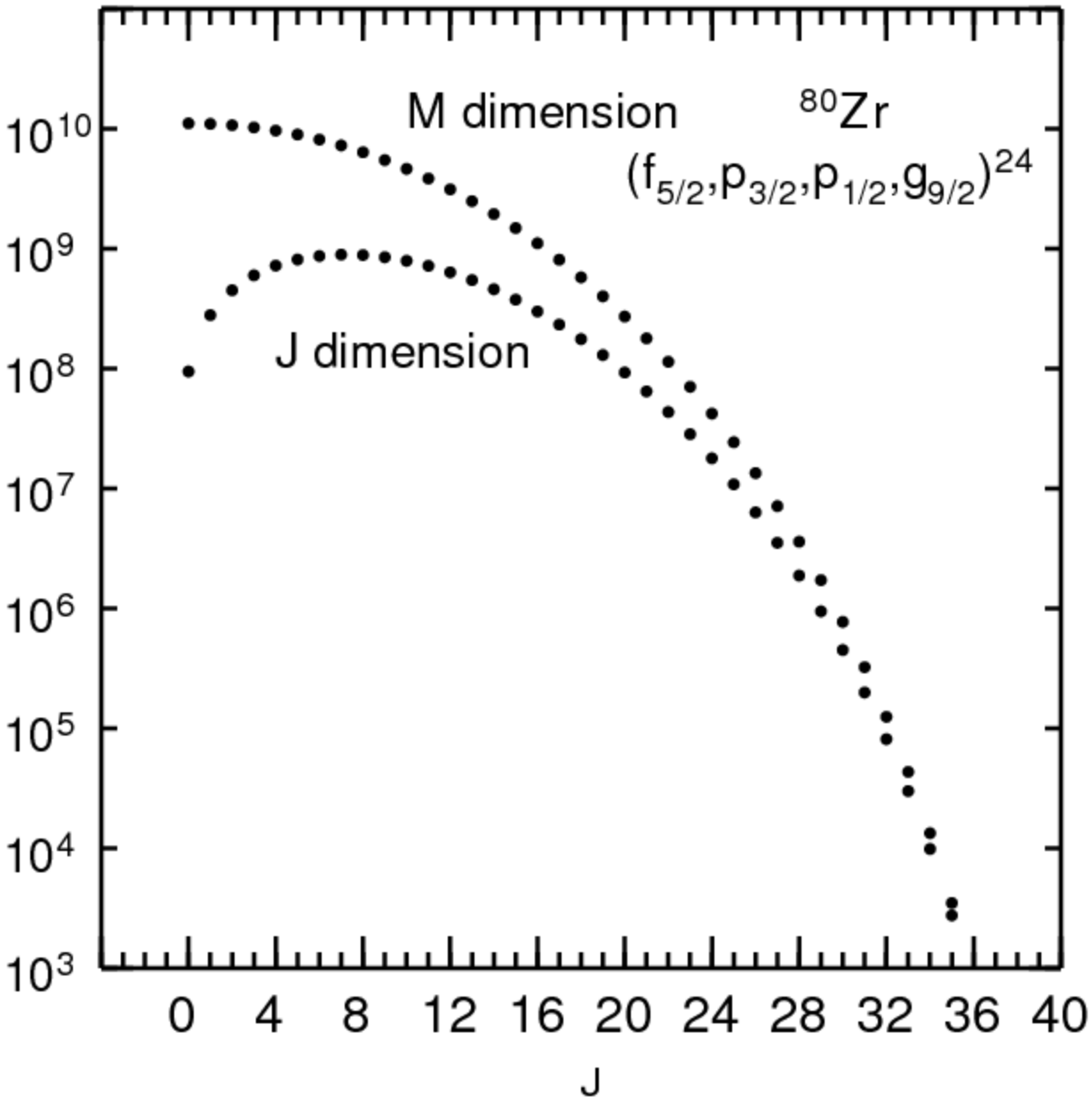
M dimension
^{80}Zr
$(f_{5/2},p_{3/2},p_{1/2},g_{9/2})^{24}$
J dimension
10^{10}
10^{9}
10^{8}
10^{7}
10^{6}
10^{5}
10^{4}
10^{3}
0 4 8 12 16 20 24 28 32 36 40
J

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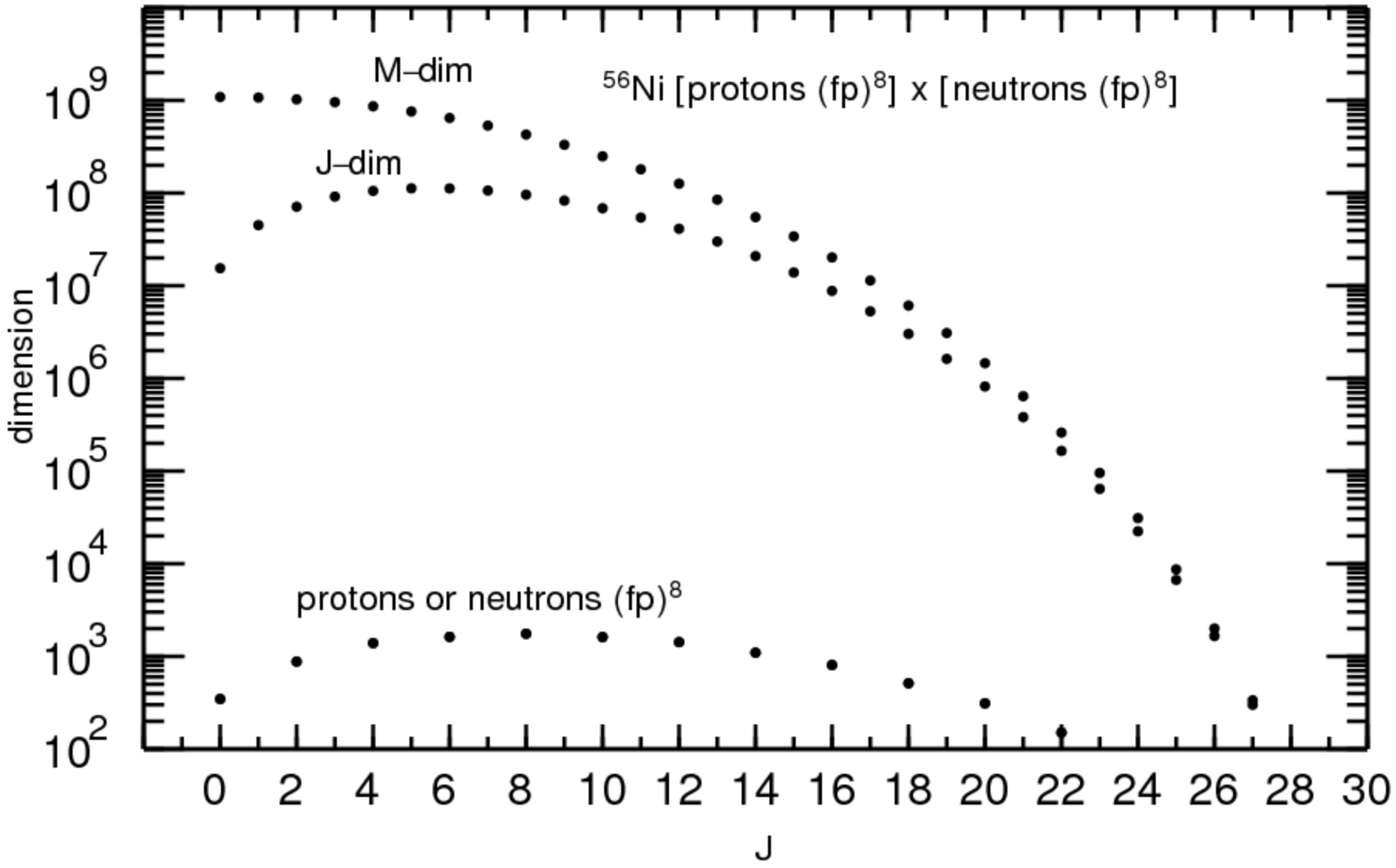
Example for ^{56}Ni in the pf shell



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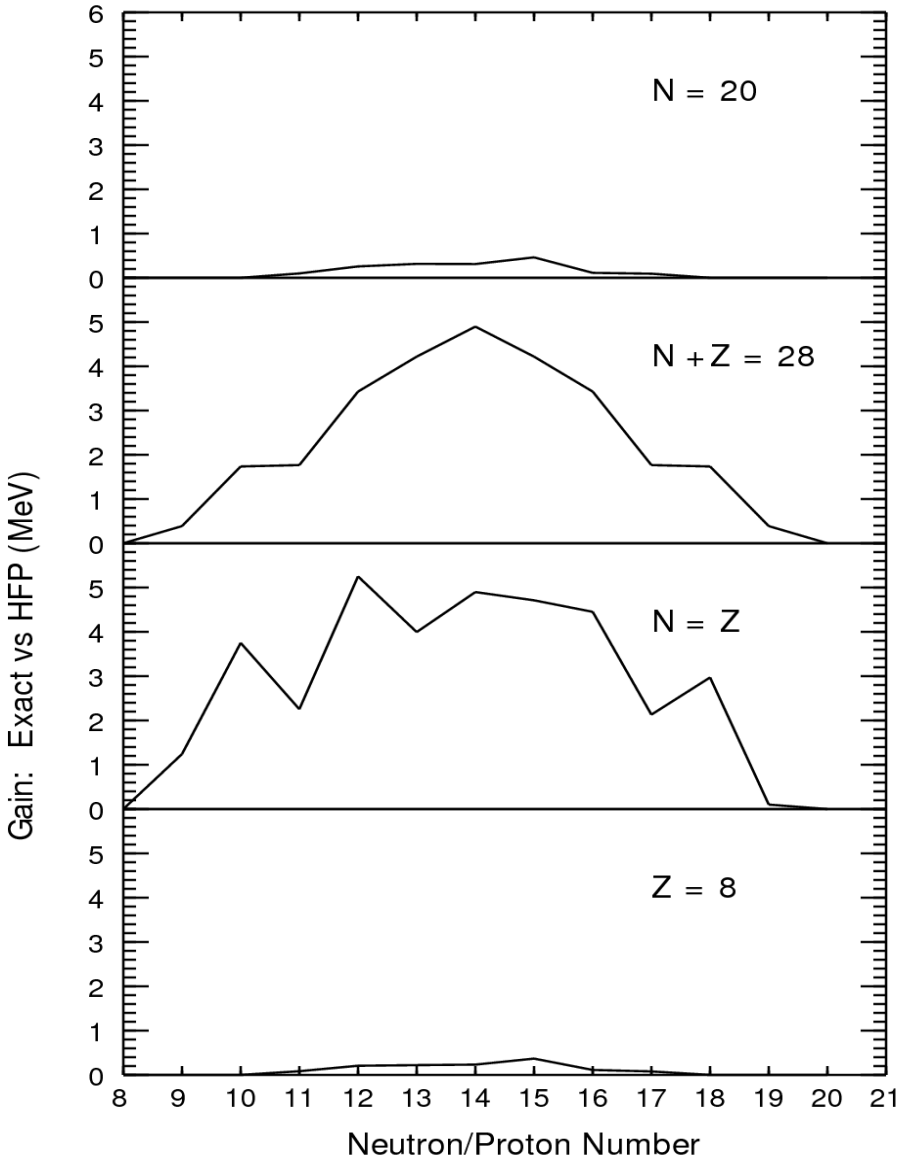
Without PN J=0, T=1 pairing



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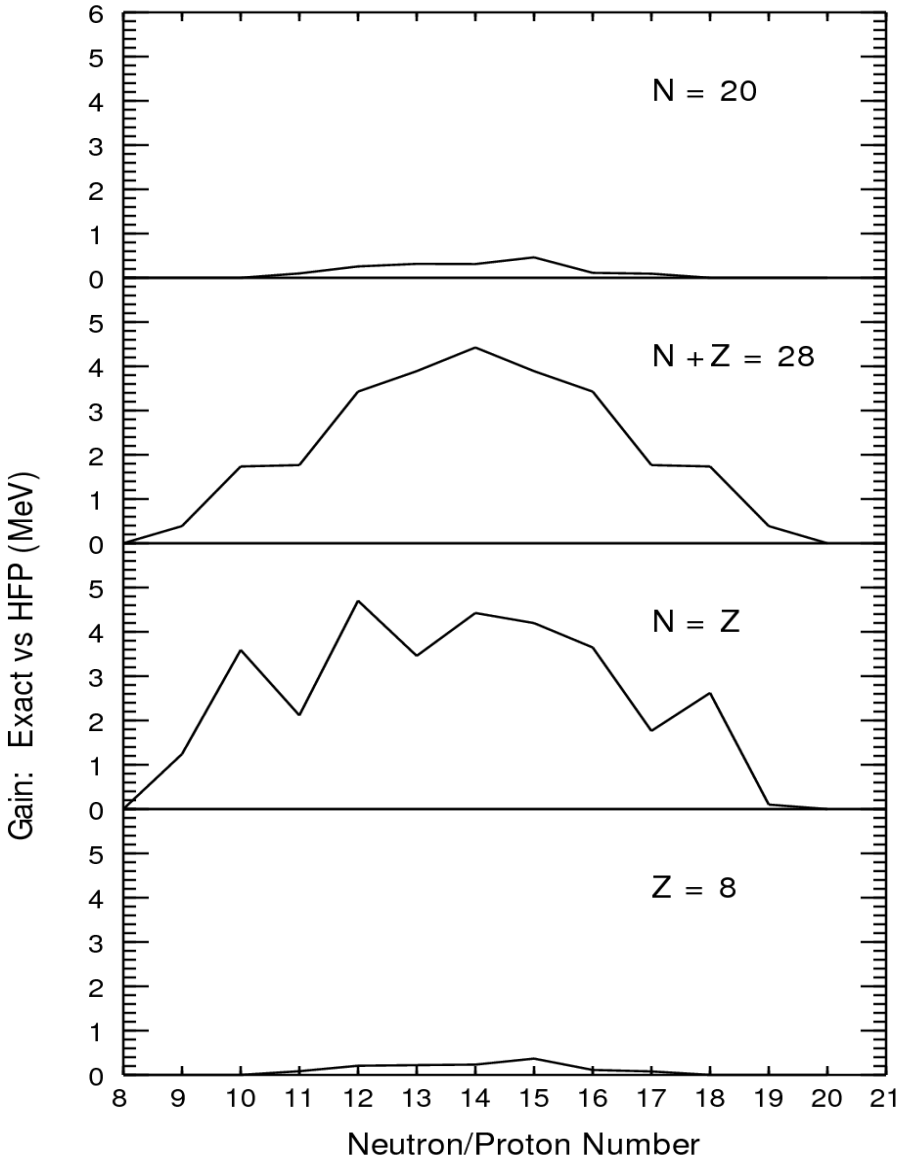
With PN J=0, T=1 pairing



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