Benchmarking theories of odd-even staggering

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Levels of theory for mass differences

1. Mean field varying only valence particle occupancies.
   Single Slater determinant (simplifed DFT).

2. Fully self-consistent mean field solutions.
   Single Slater determinant (Full DFT)

3. Multiconfiguration with pairing correlations.
   --HFB (HF+BCS in canonical basis)
   --LN
   --number-projected HFB
   --exact diagonalization

$$\Delta_o^{(3)}(N) = \frac{1}{2}\left(2E(N,Z) - E(N-1,Z) - E(N+1,Z)\right) \qquad \text{N odd}$$

Questions related to BCS

1. Dependence of $\Delta_o^{(3)}$ on $\frac{dn}{d\epsilon}, \bar{v}_{ij}, \Delta.$
2. Performance of $\Delta_o^{(3)}$
3. Evidence for induced pairing interactions?
4. Does one do better with number-conserving approximations?

Questions related to mean-field effects

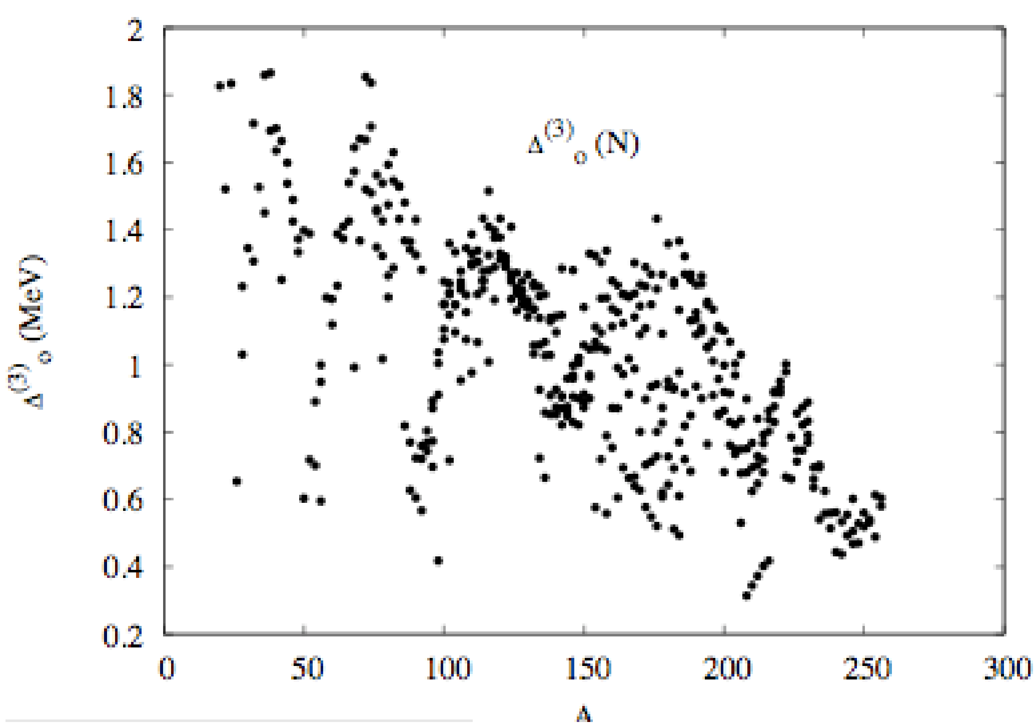
5. Are 2-body mean-field interactions adequated treated in the Skyrme DFT?
6. A-dependence?
7. Estimate of contribution from systematics?

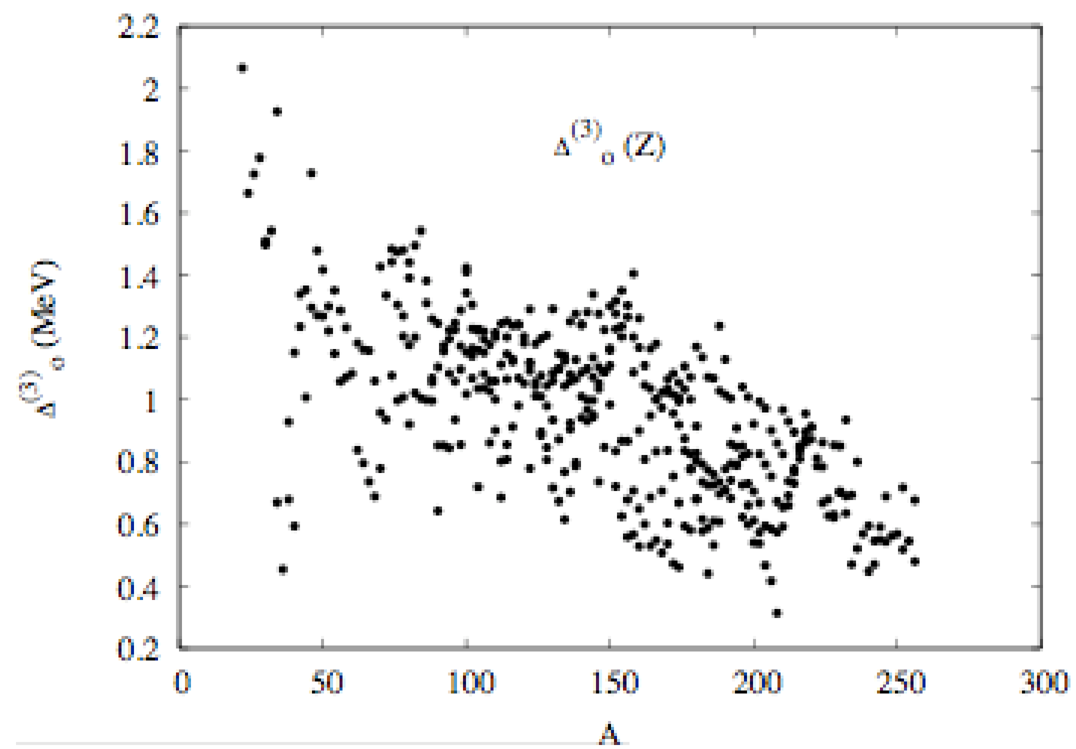
The data set

--Audi (2003) experimental mass table

-- 443 data for $\Delta_o^{(3)}(N)$ N >Z+1, Z even

-- 418 data for $\Delta_o^{(3)}(Z)$ Z < N-1, N even





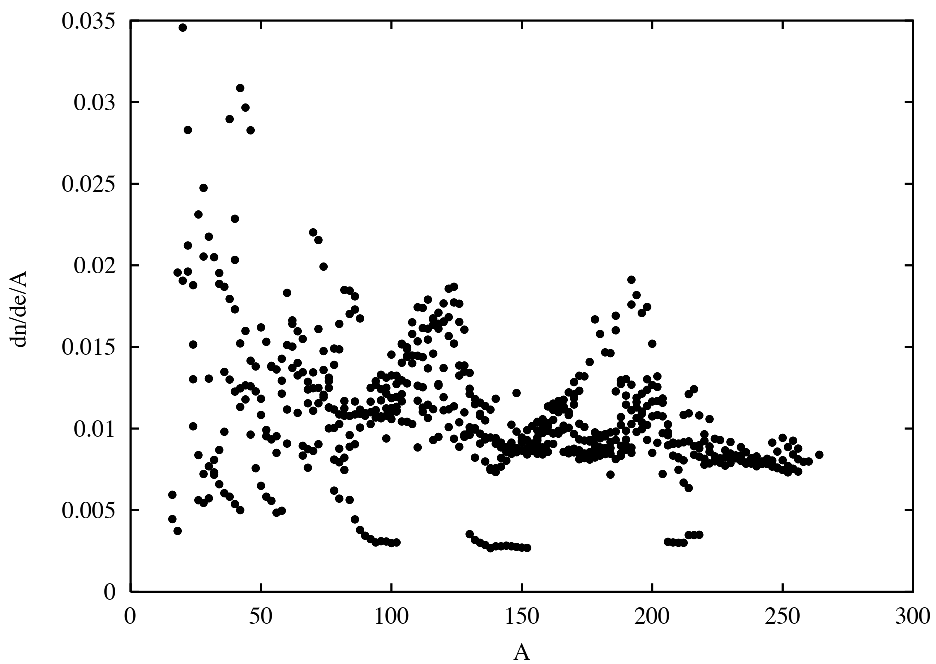
$$\Delta_o^{(3)}(N) = 1.04 \pm 0.31 \text{ MeV}$$

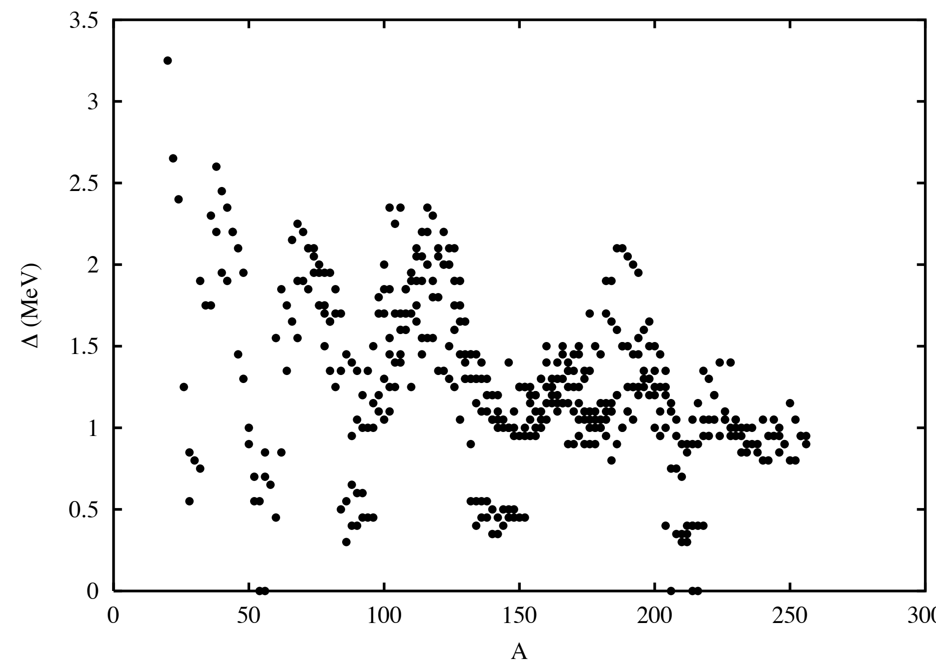
$$\Delta_o^{(3)}(Z) = 0.96 \pm 0.27 \text{ MeV}$$

BCS

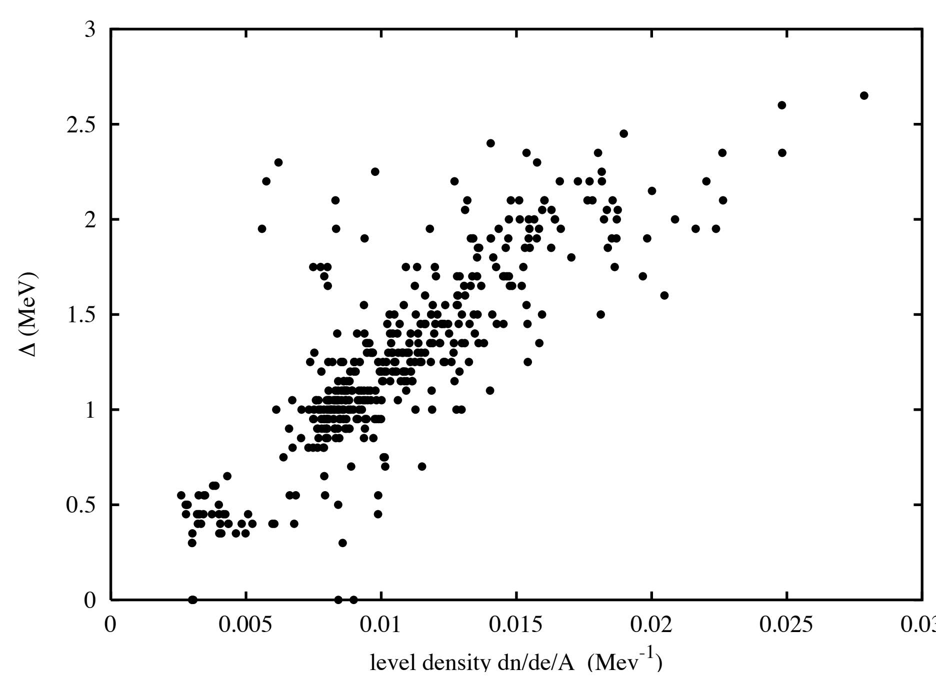
$$\Delta = E_0 \exp\left(\frac{-1}{g\frac{dn}{de}}\right) \qquad g \sim 1/A \qquad \frac{dn}{de} \sim A$$

$$\frac{dn}{de} := \frac{1}{\pi}\sum_i^{\pm 5} \frac{\delta}{(e_i - \lambda)^2 + \delta^2}$$

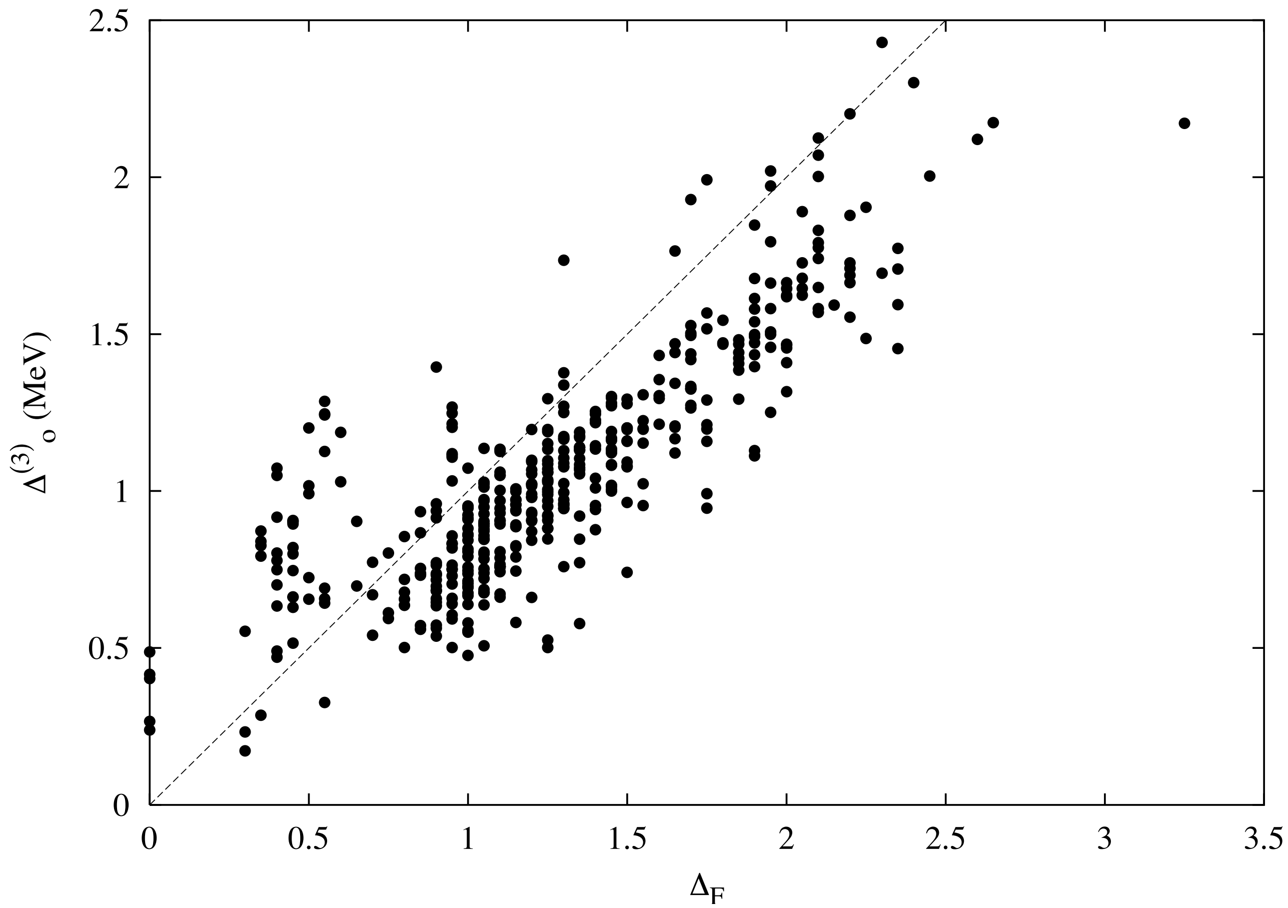


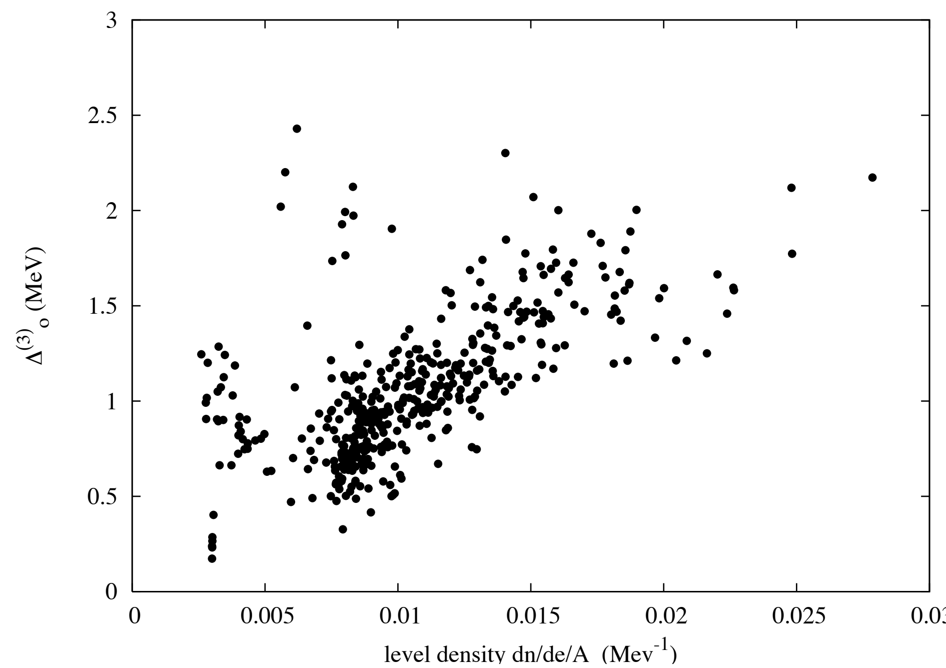


Strong correlation but there are outliers:



$$\Delta_o^{(3)} \approx \Delta$$



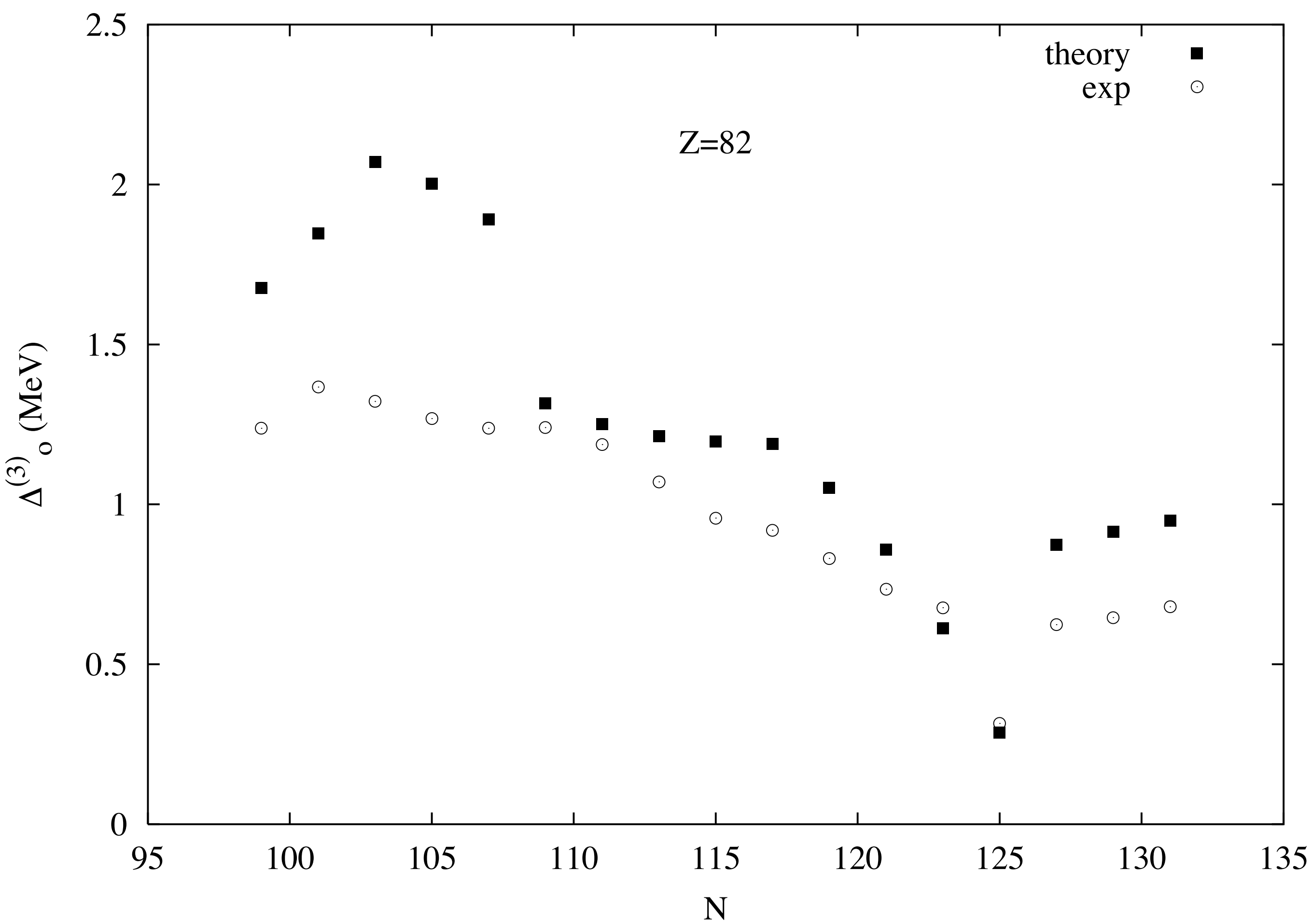


Needs to be understood:

--origin of outliers

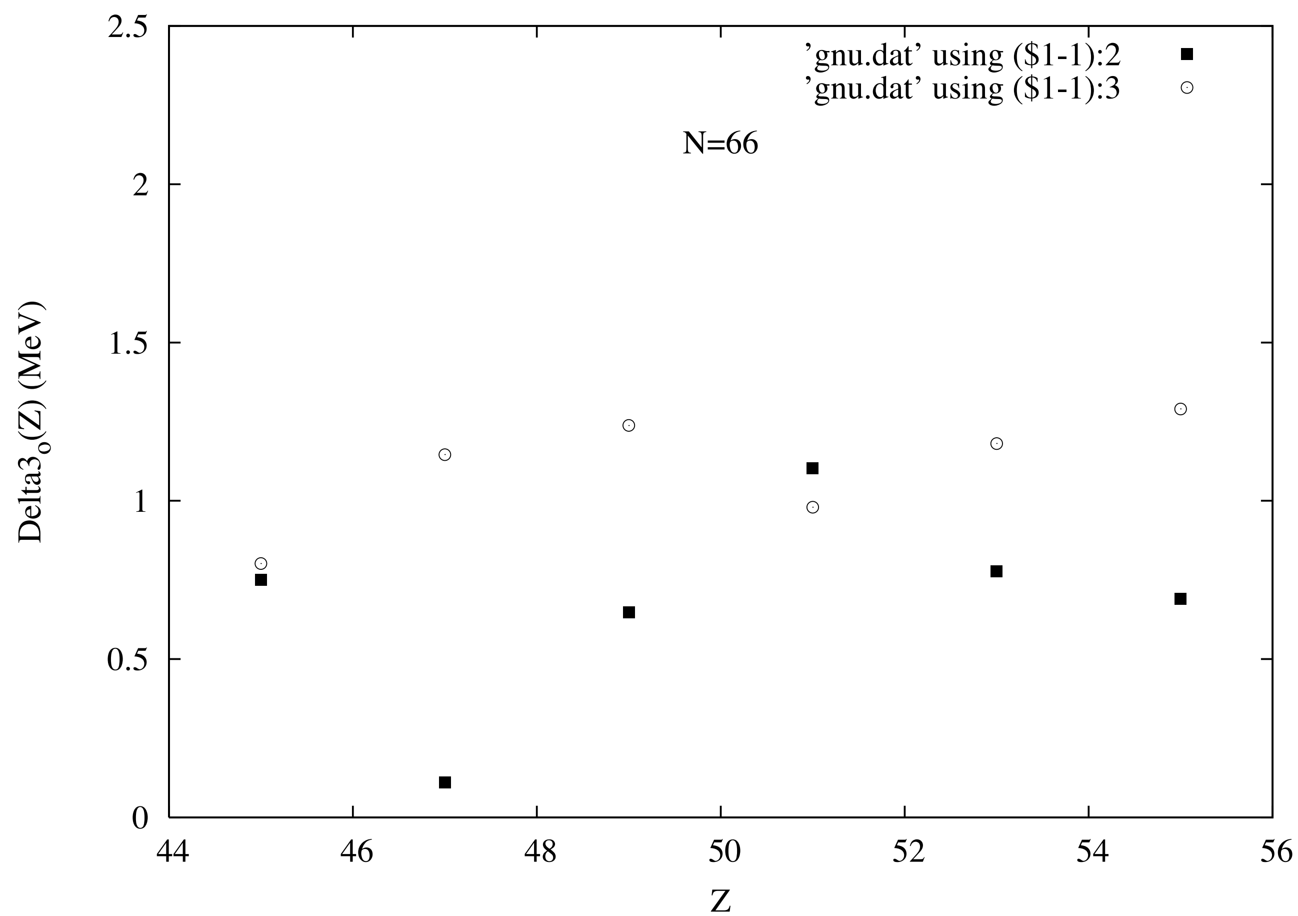
--systematic overprediction

The showcase isotope chain -- Z=82 (Pb)



On the other hand....

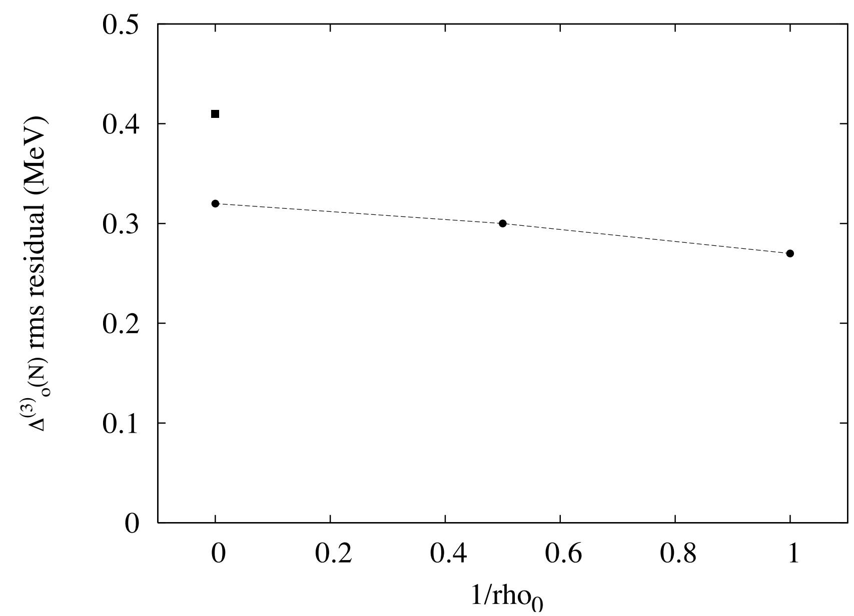
N=66



The pairing interaction

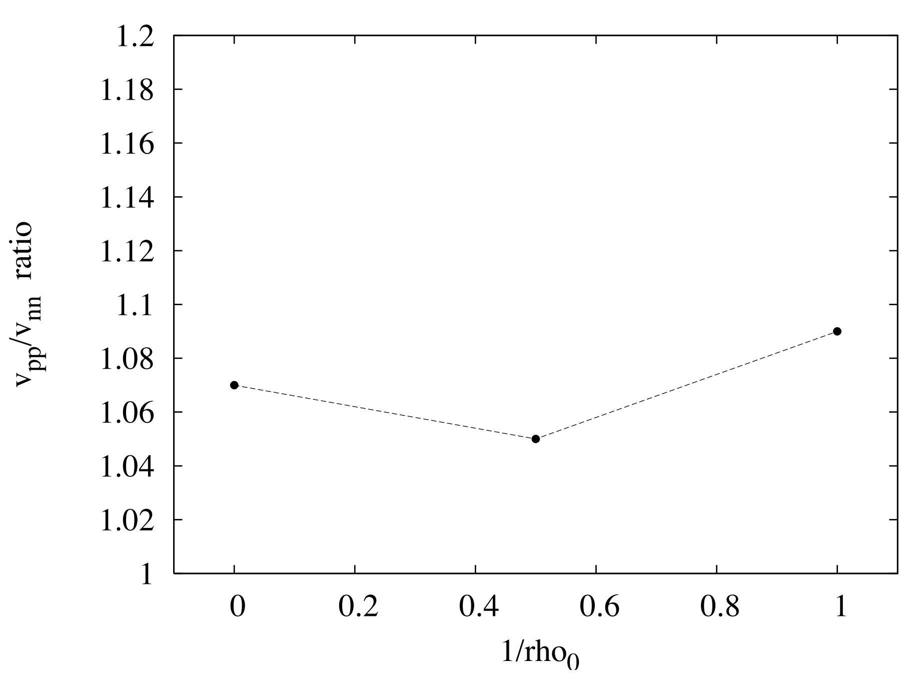
$$v_{ij} = v_0 \int d^3r |\phi_i|^2 |\phi_j|^2 (1 - \rho(r)/\rho_o)$$

Name	$1/\rho_0$ (fm^3)
v (volume)	0
m (mixed)	1/0.32
s (surface)	1/0.16



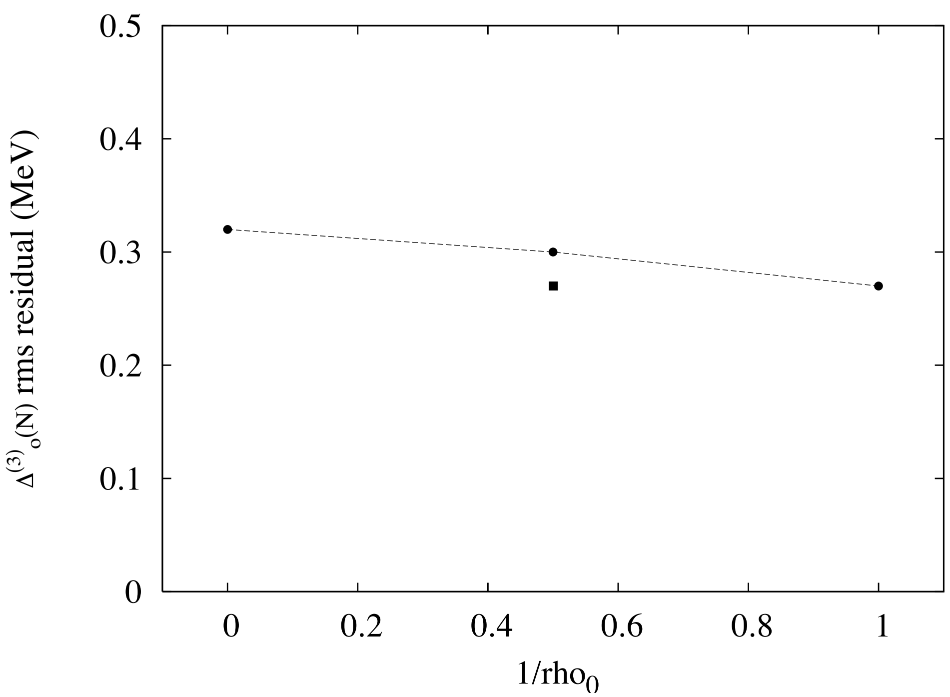
D3 is insensitive to density dependence.

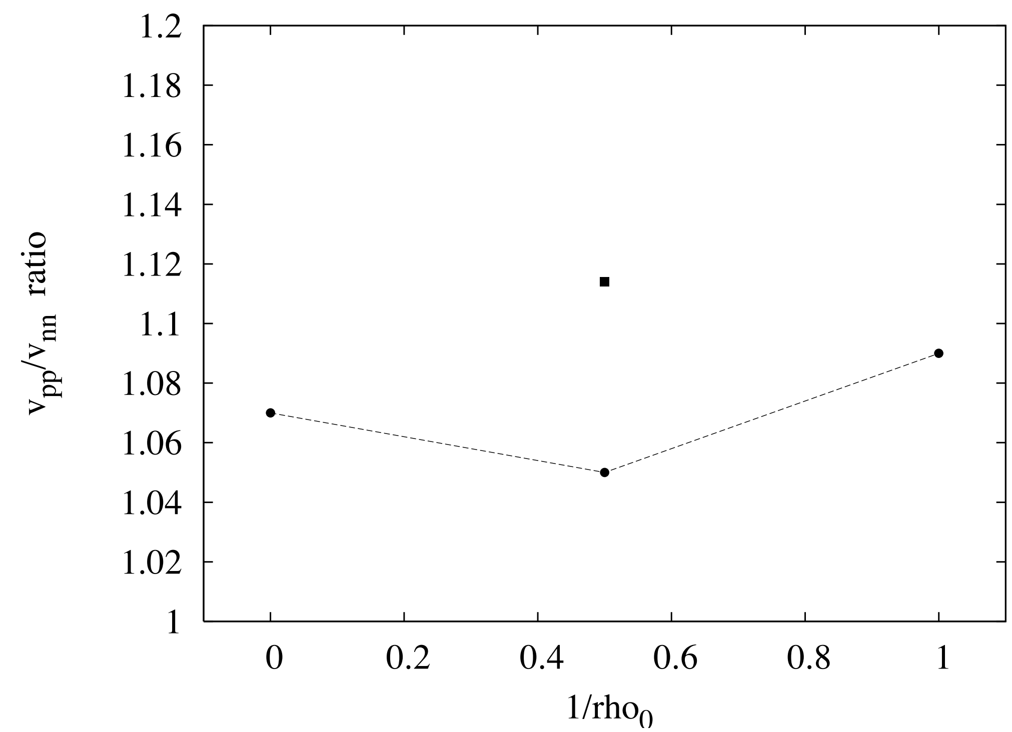
vpp /vnn



Differences are not significant except for surface pairing.

Mario's results -- using HFBTHO

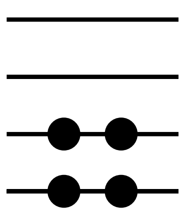




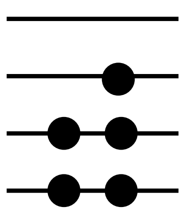
Note: HFBTHO includes mean-field effects

Understanding mean-field ("T-odd") contribution to $\Delta_o^{(3)}$

Hamiltonian formulation



even N $$V = \frac{N}{2}\bar{v}_{i\bar{i}} + \frac{N(N-2)}{2}\bar{v}_{ij}$$



odd N $$V = \left(\frac{N-1}{2}\right)\bar{v}_{i\bar{i}} + \frac{1}{2}(N-1)^2\bar{v}_{ij}$$

$\Delta_o^{(3)}$ $$-v_{i\bar{i}}/2$$

DFT formulation $\rho(r), \vec{\rho}_\sigma(r)$

$$V = v_0 \int \rho^2 d^3r + v_\sigma \int \vec{\rho}_\sigma \cdot \vec{\rho}_\sigma d^3r$$

even N $$\int \rho \, d^3r = N; \;\; \vec{\rho}_\sigma = 0$$

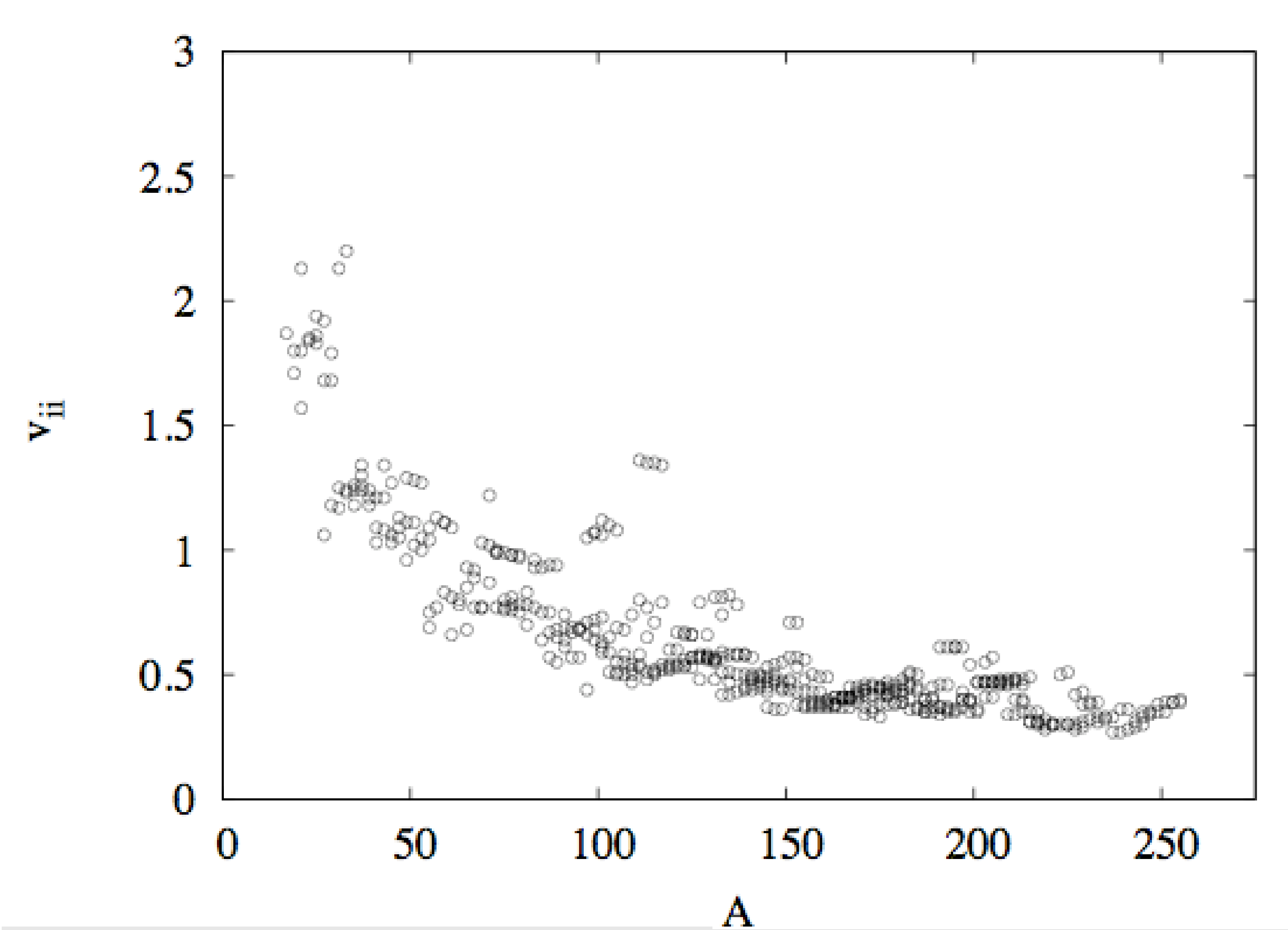
$$V = v_0 \int \rho^2 \, d^3r \approx \frac{v_0}{\Omega} N^2$$

odd N $$\vec{\rho}_\sigma(r) = \vec{n}(r)\rho_i(r); \;\; \int \rho_i \, d^3r = 1$$

$$V = \frac{v_0}{\Omega} N^2 + v_\sigma \int \rho_i^2 \, d^3r$$

$\Delta_o^{(3)}$ $$v_\sigma \int \rho_i^2 \, d^3r \approx \frac{v_\sigma}{\Omega} \sim \frac{1}{N}$$

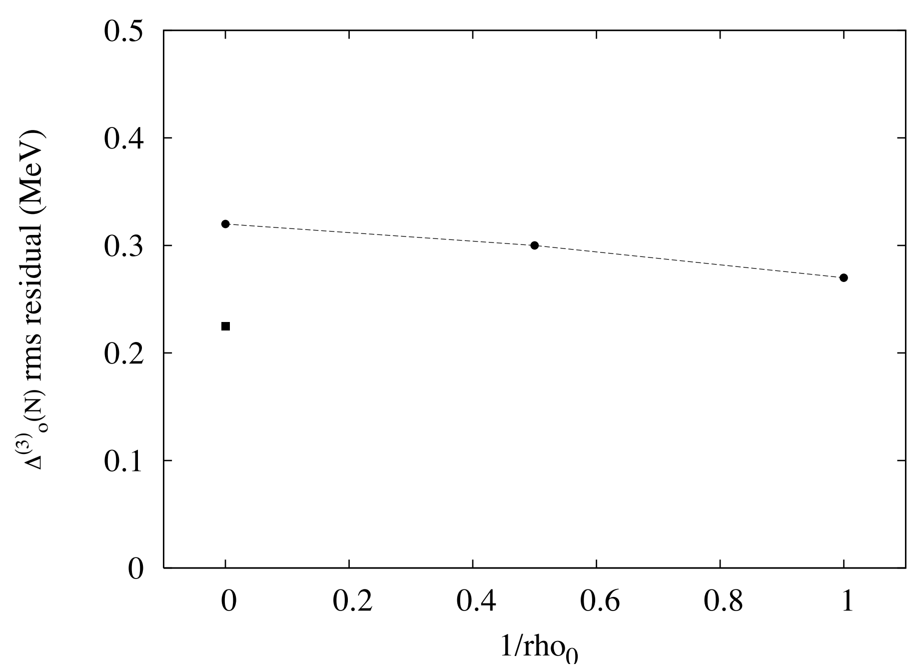
Systematics of $\int \rho_i^2 \, d^3 r$



How important is the v_sigma term? A question to Dick, but we can get a preview by fitting.

Fit to

$$x\Delta_o^{(3)}(BCS) + (1-x)\int \rho_i^2\, d^3r$$



There is hope for major improvement!

Questions

1. Year 2 plans on track?

Bertsch (UW)

I will test extensions of the DFT using shell-model Hamiltonians to simulate the actual Hamiltonian. I hope this will help to understand the disagreement between methods using the GCM to calculate spectroscopic properties. This work will be done with Brown (MSU). I will also work with Bertulani (TAMU) to evaluate the systematic performance of the simpler treatments of pairing in odd-A systems. This will be done with the codes EV8 (BCS) and CR8 (HFB) from Heenen (Bruxelles). The results will provide a base to compare with the more thorough theory being carried out by the UT/ORNL group.

GCM: 30%
Pairing: 100% by Yr2 end

2. High-performance computing?

Not in Yr3

3. Computational issues?

Solvers for nonlocal functionals

4. Detailed roadmap?

Finish up pairing survey, including exact pairing

Explore effects of finite-range nonlocality

S_nn for isotone chains

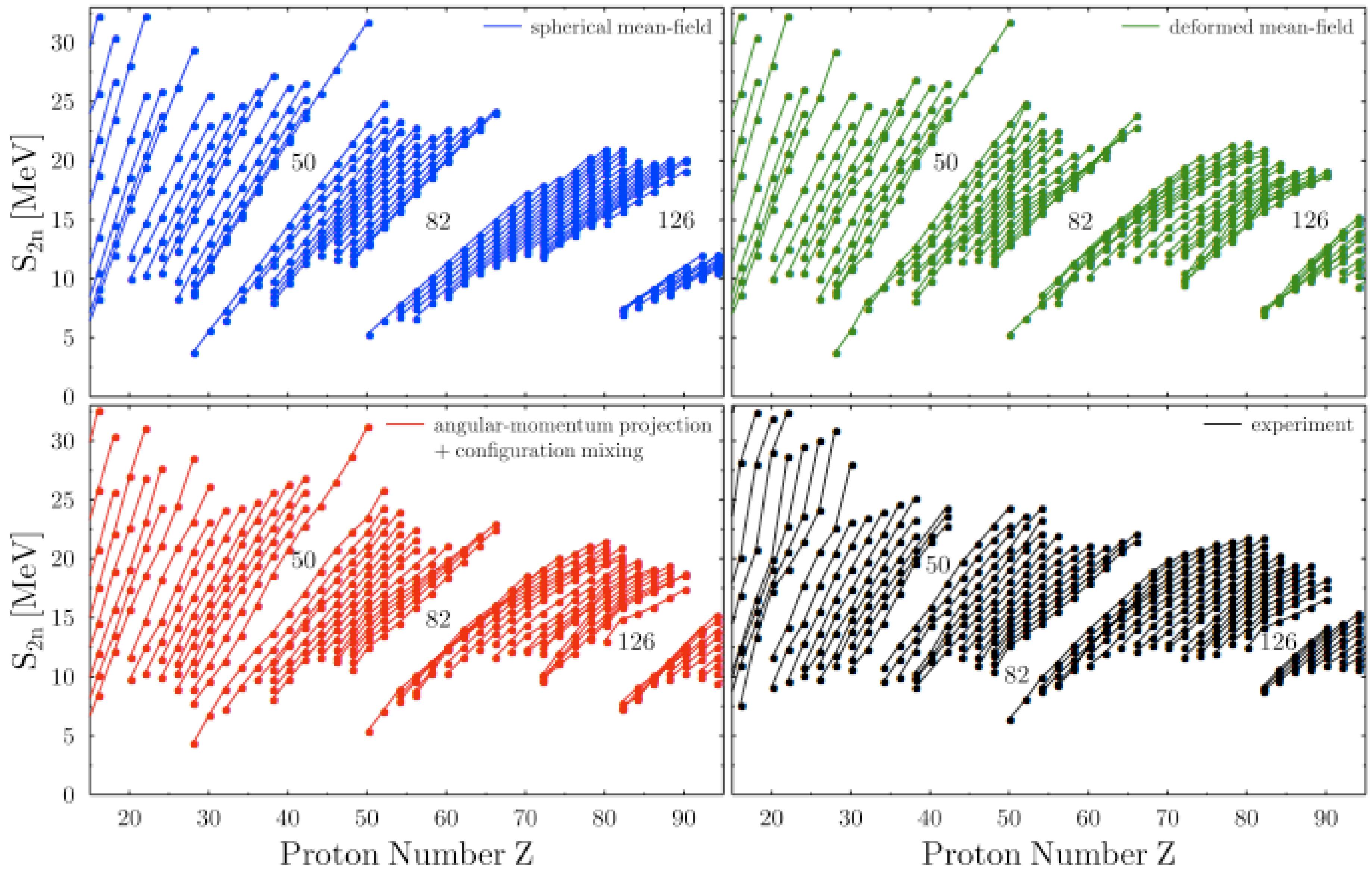


FIG. 1: Two-neutron separation energies for isotonic chains. We compare results obtained from three calculations (i) spherical mean field. (ii) deformed mean field (iii) $J = 0$ projected axial quadrupole GCM with the experiment.