Extension of mean-field theory for spectroscopy

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INT-11-3
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0. Quantities calculated
1. Generalities
2. Performance assessment
3. Theories considered
4. Results

Quantities calculated

Low-lying excitations:
- 2+
- 3-

Yrast levels
Charge radii
Separation energies
Pairing gaps

Bibliography

G.F. Bertsch, C.A. Bertulani, W. Nazarewicz, N. Schunck, and M. Stoitsov, PR C 79 034306 (2009).

J.P. Delaroche, M. Girod, J. Libert, H. Goutte, S. Hilaire, S. Peru, N. Pillet, G.F. Bertsch, PRC 81 014303 (2010).

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L.M. Robledo and G.F. Bertsch, arXiv:1107.3581

Generalities

Characteristics of good theories

- -need only a small set of parameters
- -have wide predictive power
- -have intrinsic criteria for limits of validity

Goals in this work

- -apply theory globally (but with exceptions...)
- -quantitative assessment of performance
- -predictions to be tested by FRIB and elsewhere

Performance Metric:

Mean error and rms deviation about the mean, on a logarithmic scale.

$$R_i = \log\left(\frac{x^i_{th}}{x^i_{exp}}\right)$$

$$\bar{R} = \frac{1}{N}\sum_i^N R_i$$

$$\sigma_x \equiv \langle (R_x - \bar{R}_x)^2 \rangle^{1/2}.$$

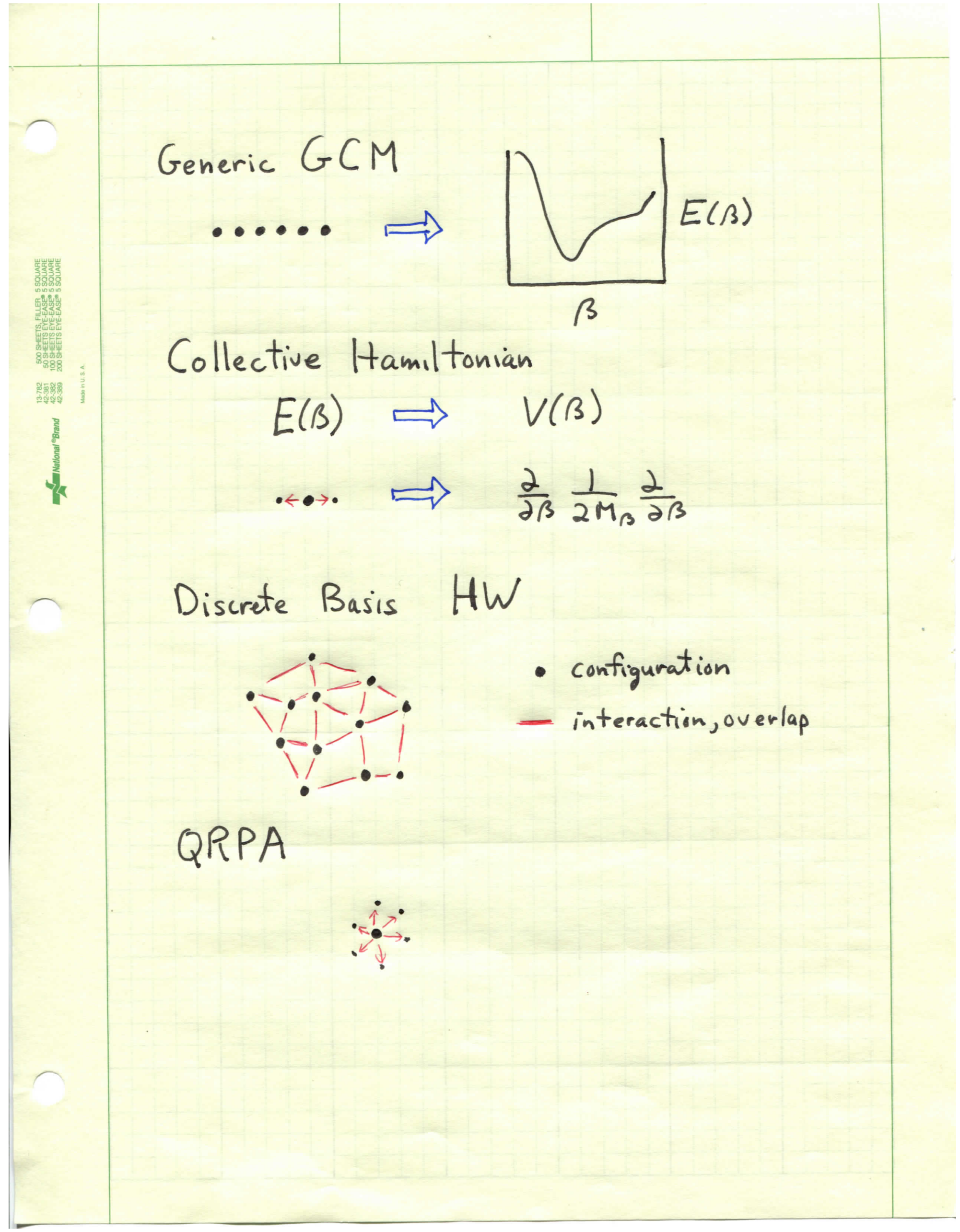
Extensions of self-consistent mean-field theory for spectroscopy

Generator Coordinate Methods

Collective Hamiltonian
GOA

Discrete-basis Hill-Wheeler

Quasiparticle RPA



How to do GCM

$\hat{H}$ = the many-body Hamiltonian, usually approximated by an EDF.

$\hat{Q}_i$ = a set of one-body operators

I) Minimize $\langle \psi_\lambda | \hat{H} - \sum_i \lambda_i \hat{Q}_i | \psi_\lambda \rangle$ to find ψ_λ

II find expectation values $q_i = \langle \psi_\lambda | \hat{Q}_i | \psi_\lambda \rangle$

$$V(q) \equiv V(\lambda(q)) = \langle \psi_\lambda | \hat{H} | \psi_\lambda \rangle$$

This is the potential energy surface.

5DCH work: $\hat{N}, \hat{Z}, r^2 Y_{20}, r^2 Y_{2\pm2}, \hat{J}_x$

octupole study: $\hat{N}, \hat{Z}, r^2 Y_{20}, r^3 Y_{30}$

The CEA/DAM global survey (HFB/GCM/5DCH)

PRC 81, 014303 (2010)

Abstract | References | Citing Articles (8) | **Supplemental Material**

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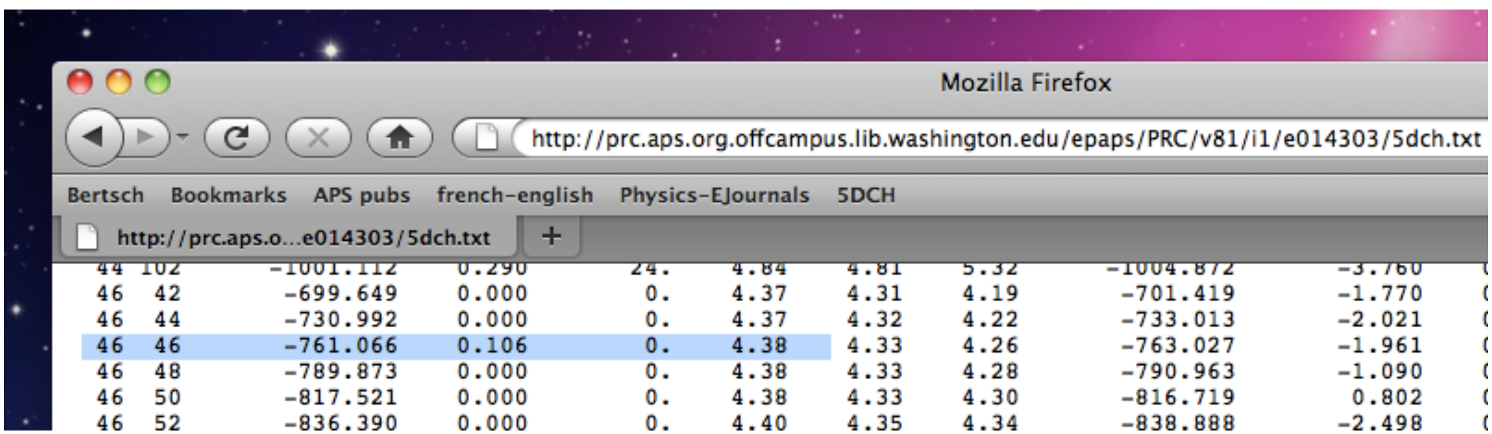
EPAPS

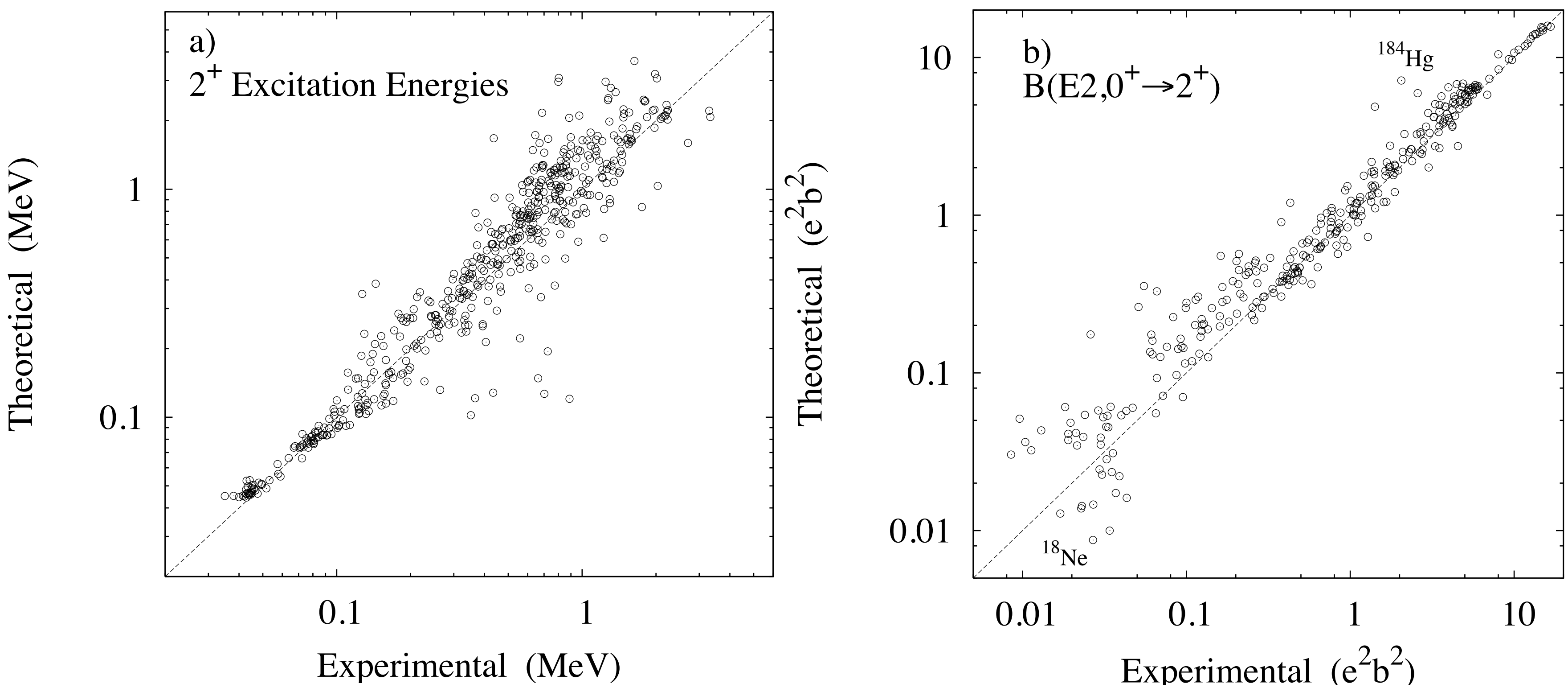
- README.TXT
- 5dch.txt
- heading_5dch-table-eng.doc

Computed spectroscopic observables for 1712 nuclei:
- -yrast energies up to J=6
- -excited 0+, first and second yrare J=2
- -B(E2) values for many of the transitions
- -E0 matrix elements
- -deformations, including triaxiality



44	102	-1001.112	0.290	24.	4.84	4.81	5.32	-1004.872	-3.760
46	42	-699.649	0.000	0.	4.37	4.31	4.19	-701.419	-1.770
46	44	-730.992	0.000	0.	4.37	4.32	4.22	-733.013	-2.021
46	46	-761.066	0.106	0.	4.38	4.33	4.26	-763.027	-1.961
46	48	-789.873	0.000	0.	4.38	4.33	4.28	-790.963	-1.090
46	50	-817.521	0.000	0.	4.38	4.33	4.30	-816.719	0.802
46	52	-836.390	0.000	0.	4.40	4.35	4.34	-838.888	-2.498

Global assessment of accuracy: first excited J=2 state



E(exp) = E(theory)+/-40% over 2 order of magnitude

Many other observables

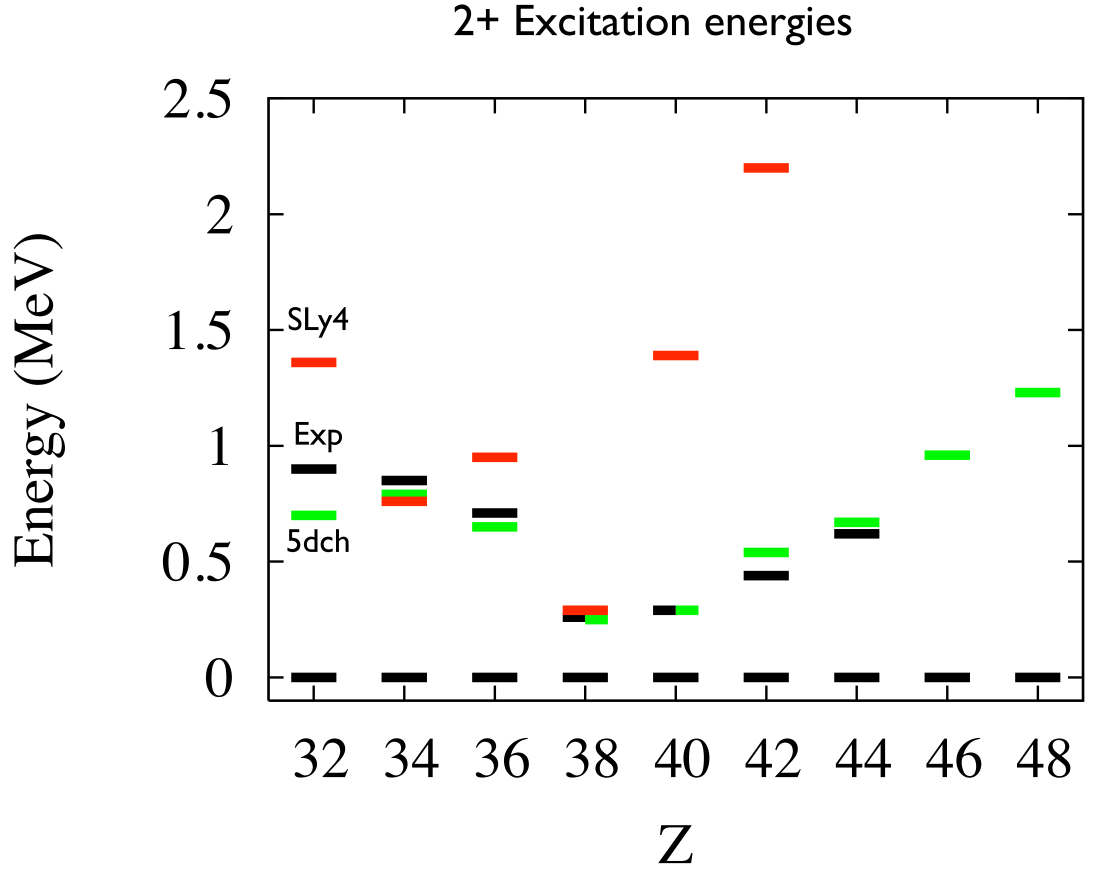
Metrics for global performance

$$R_i = \log\left(\frac{x^i_{th}}{x^i_{exp}}\right) \qquad \sigma_x \equiv \langle (R_x - \bar{R}_x)^2 \rangle^{1/2}.$$

Observable	Number	$\bar{R}$	σ
$E(2_1^+)$	513	0.11	0.35
$B(E2; 2_1^+ \to 0_1^+)$	311	0.20	0.42
R_{42}	480	0.03	0.14
R_{62}	427	0.08	0.21
$E(2_2^+)$	352	0.19	0.30
$E(0_2^+)$	317	0.31	0.36
$\langle 0_2^+ \| r_p^2 \| 0_1^+ \rangle$	87	2.1	1.9

The CEA/DAM global survey (HFB/GCM/5DCH), on the N=Z line

PRC 81, 014303 (2010)



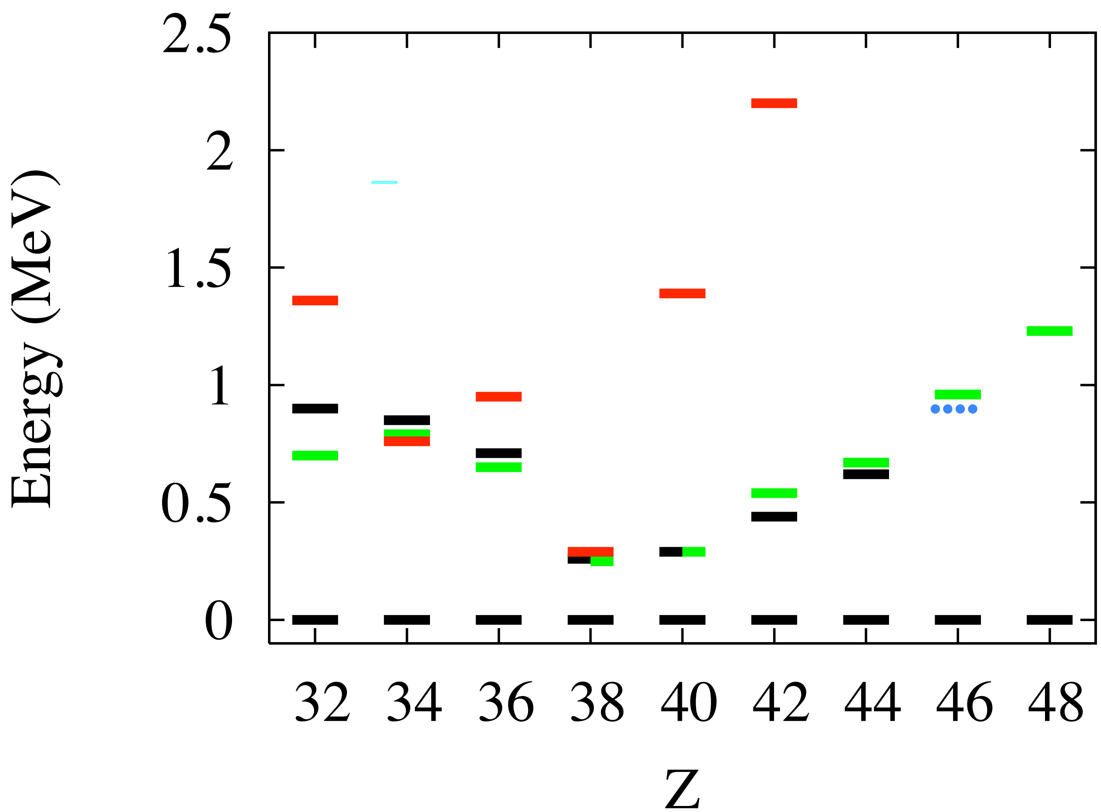
LETTER

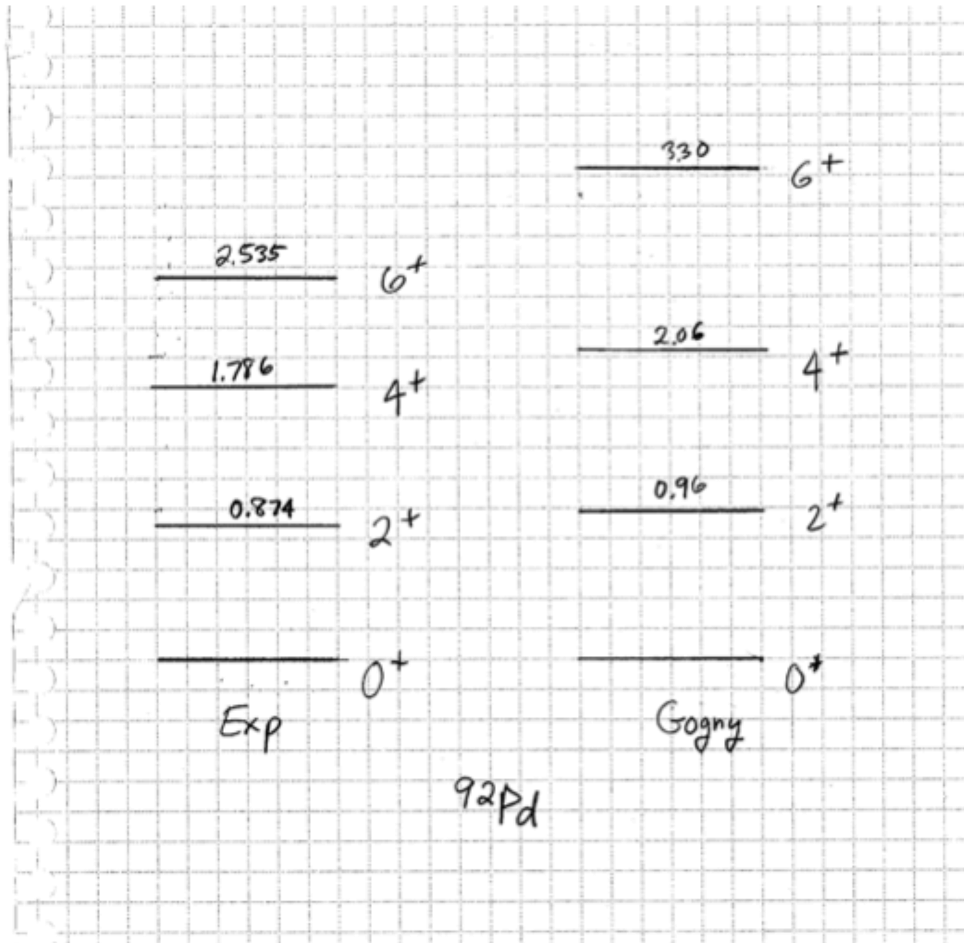
Nature 469 68 (2011)

doi:10.1038/nature09644

Evidence for a spin-aligned neutron–proton paired phase from the level structure of ^{92}Pd

B. Cederwall[1], F. Ghazi Moradi[1], T. Bäck[1], A. Johnson[1], J. Blomqvist[1], E. Clément[2], G. de France[2], R. Wadsworth[3], K. Andgren[1], K. Lagergren[1,4], A. Dijon[2], G. Jaworski[5,6], R. Liotta[1], C. Qi[1], B. M. Nyakó[7], J. Nyberg[8], M. Palacz[5], H. Al-Azri[3], A. Algora[9], G. de Angelis[10], A. Ataç[11], S. Bhattacharyya[2]†, T. Brock[3], J. R. Brown[3], P. Davies[3], A. Di Nitto[12], Zs. Dombrádi[7], A. Gadea[9], J. Gál[7], B. Hadinia[1], F. Johnston-Theasby[3], P. Joshi[3], K. Juhász[13], R. Julin[14], A. Jungclaus[15], G. Kalinka[7], S. O. Kara[11], A. Khaplanov[1], J. Kownacki[5], G. La Rana[12], S. M. Lenzi[16], J. Molnár[7], R. Moro[12], D. R. Napoli[10], B. S. Nara Singh[3], A. Persson[1], F. Recchia[16], M. Sandzelius[1]†, J.-N. Scheurer[17], G. Sletten[18], D. Sohler[7], P.-A. Söderström[8], M. J. Taylor[3], J. Timár[7], J. J. Valiente-Dobón[10], E. Vardaci[12] & S. Williams[19]

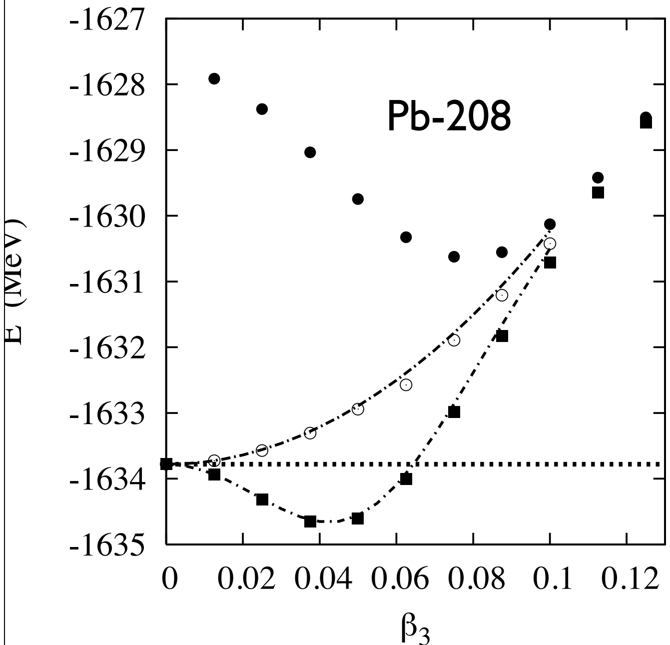


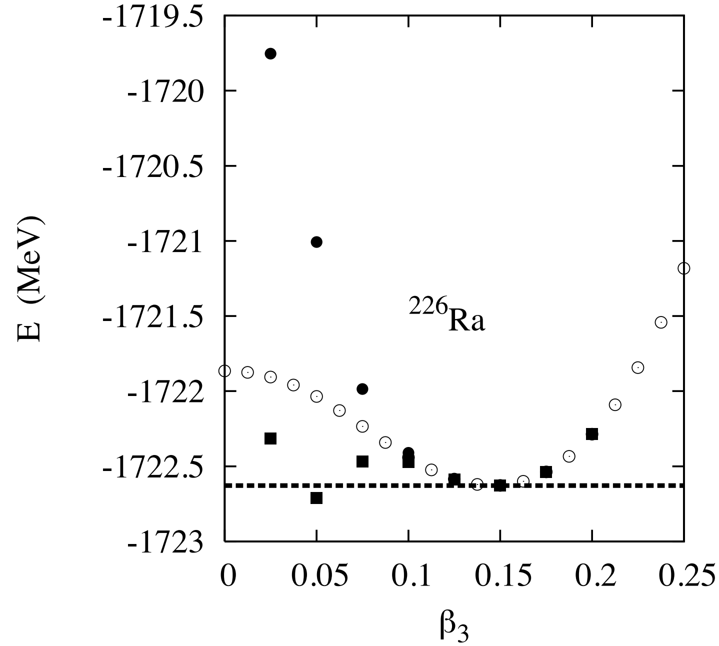

2.535
6+
1.786
4+
0.874
2+
0+
Exp
3.30
6+
2.06
4+
0.96
2+
0+
Gogny
92Pd

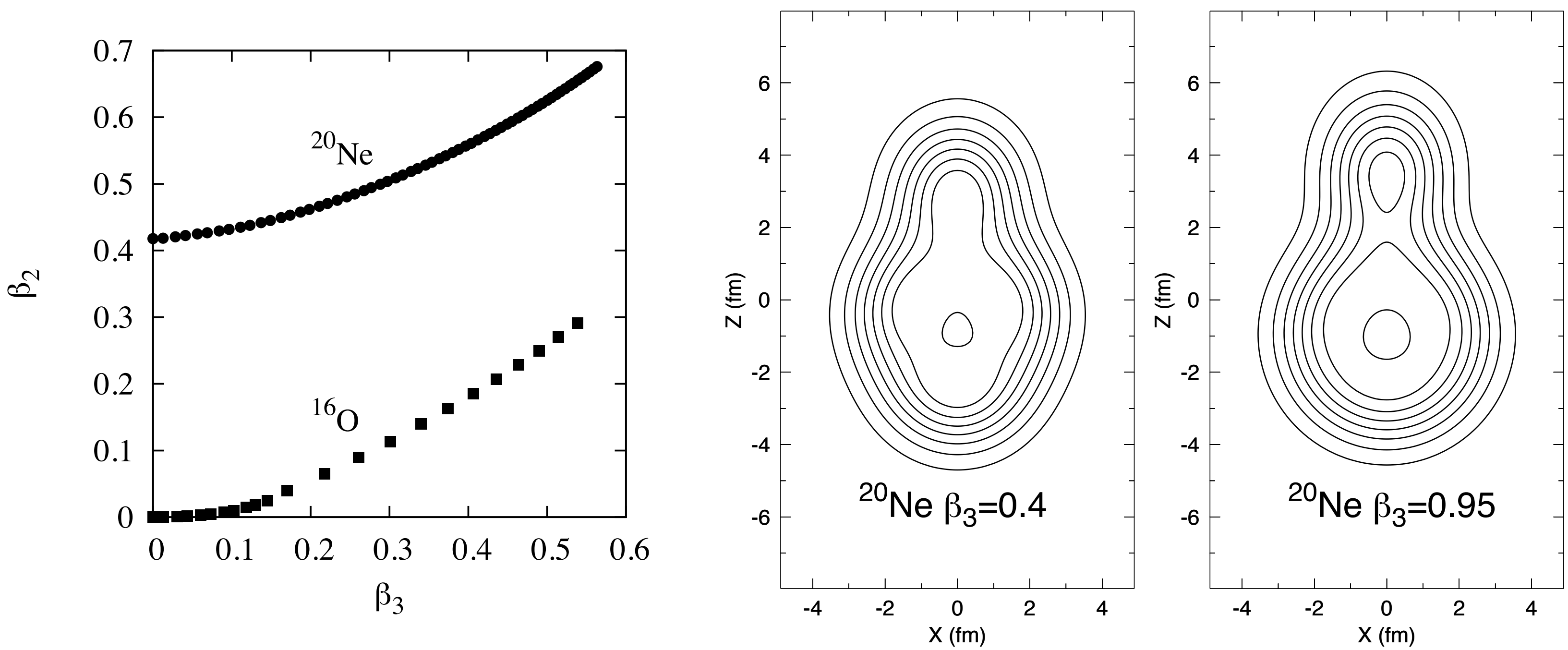
Octupole Excitations

Robledo and Bertsch, arXiv:1107.3581
HFB + discrete basis Hill-Wheeler
Parity projection
Axially symmetric octupole excitations only.

Examples of energy surfaces

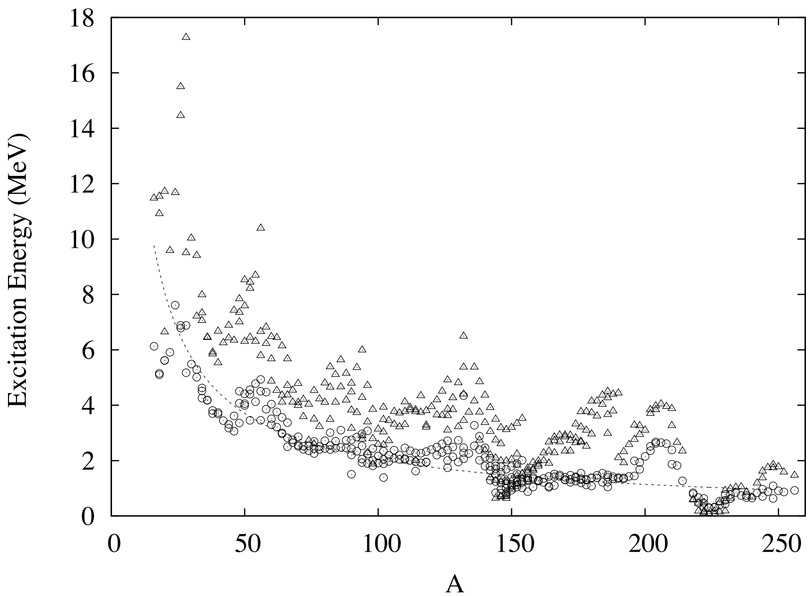


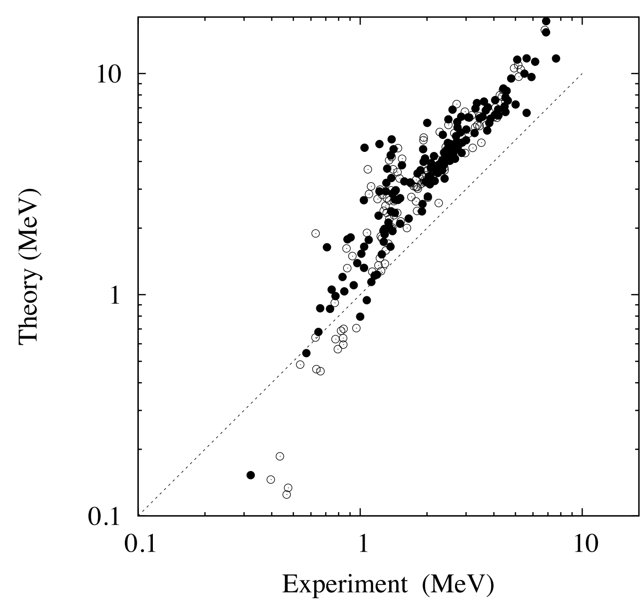




0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0 0.1 0.2 0.3 0.4 0.5 0.6
β_2
β_3
^{20}Ne
^{16}O
6
4
2
0
-2
-4
-6
-4 -2 0 2 4
Z (fm)
X (fm)
^{20}Ne β_3=0.4
^{20}Ne β_3=0.95

3- excitation energies



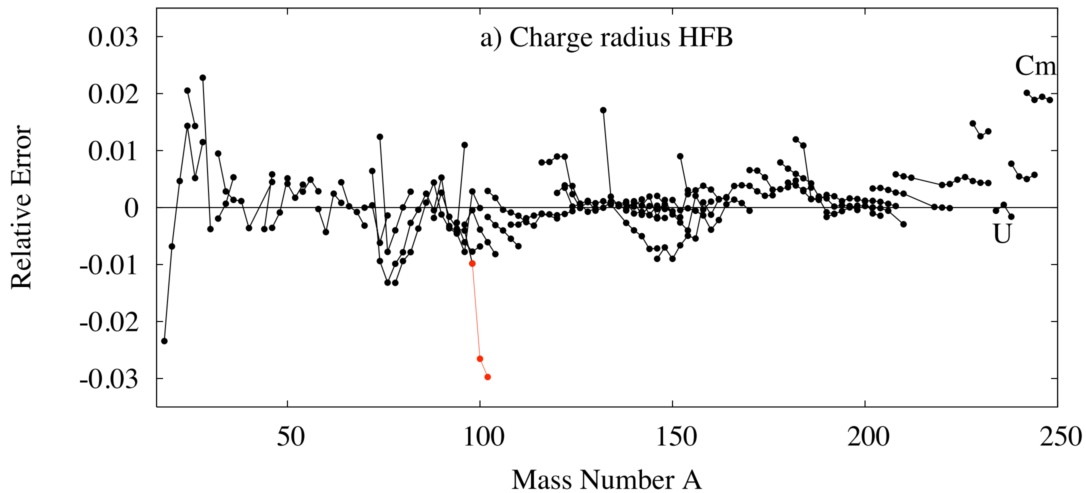


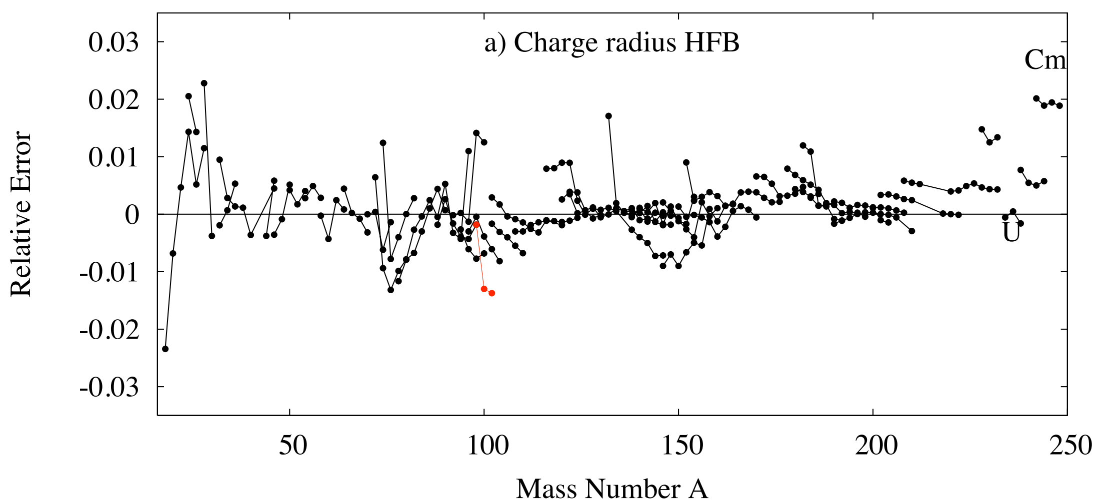
		HW		MAP	
Selection	Number	R_e	σ_e	R_e	σ_e
all	284	0.45	0.40		
$\beta_3 = 0$	277	0.55	0.23	0.59	0.22
$\beta_3 = 0$, def.	59	0.62	0.32	0.75	0.26
$\beta_3 = 0$, sph.	196	0.52	0.19	0.53	0.17

Charge radii

Experimental data from Angeli, ADNDT 87 (2004)

HFB





Performance on charge radius

TABLE II. Comparison of calculated charge radii with experiment: $\bar{\epsilon}$ is the mean of ϵ [see Eq. (18)]; σ is its rms dispersion about the average. Three hundred thirteen nuclear radii were included in the comparison as in Fig. 6. In the column "HFB (new)" we use the modern value $r_p = 0.875$ fm for the proton charge radius [48].

Theory	R	σ
HFB	0.001	0.006
HFB (new)	0.005	0.007
CHFB+5DCH	0.006	0.007
Finite surface	0.0000	0.012

Separation Energies

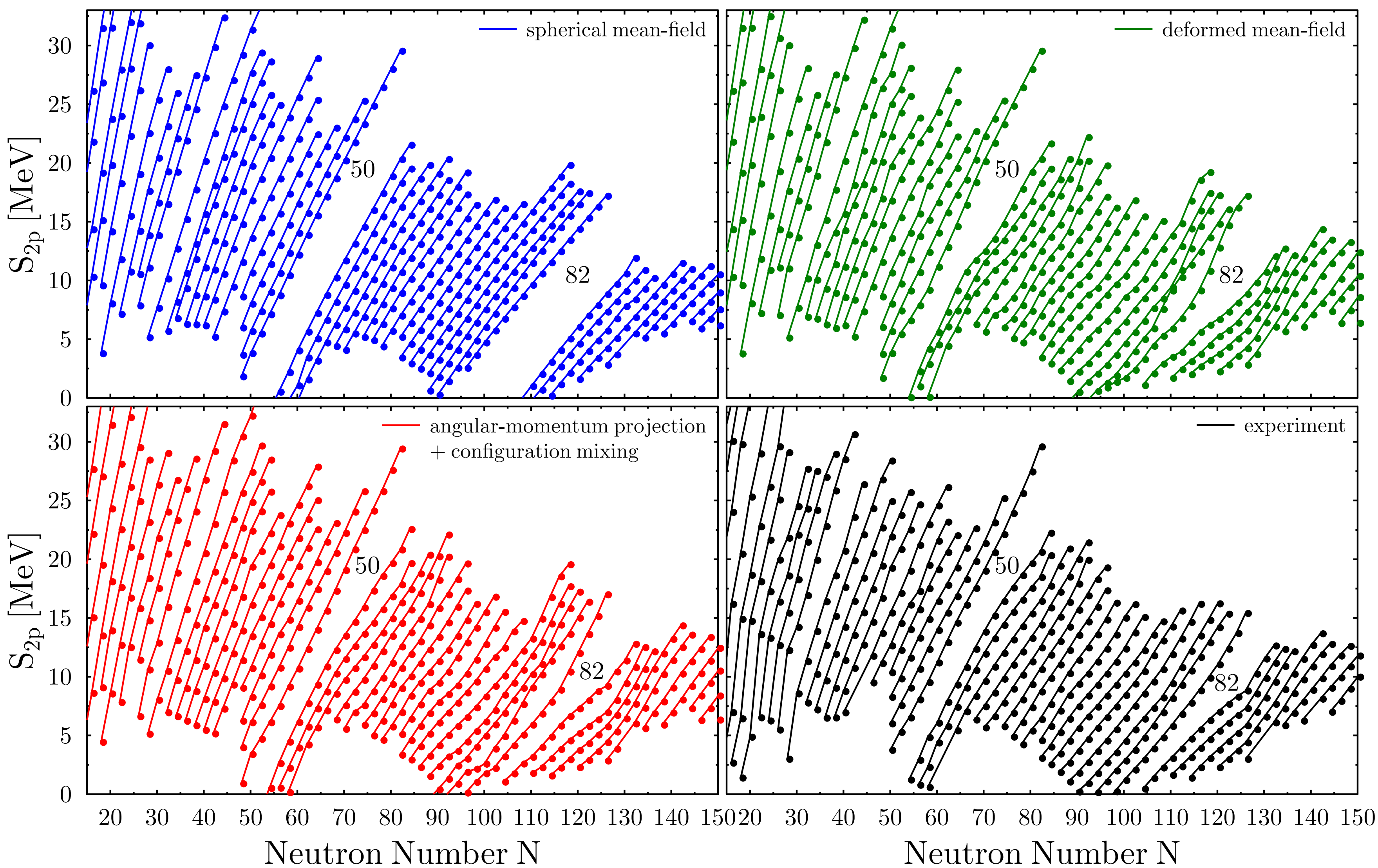


FIG. 2: Two-proton separation energies for isotonic chains.

Mutually enhanced magicity

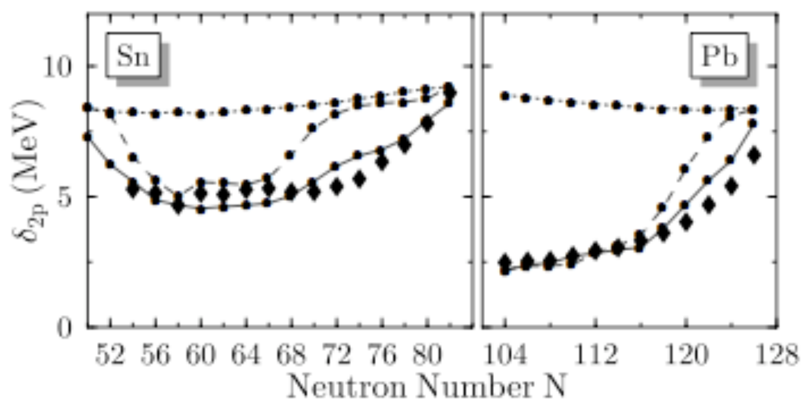
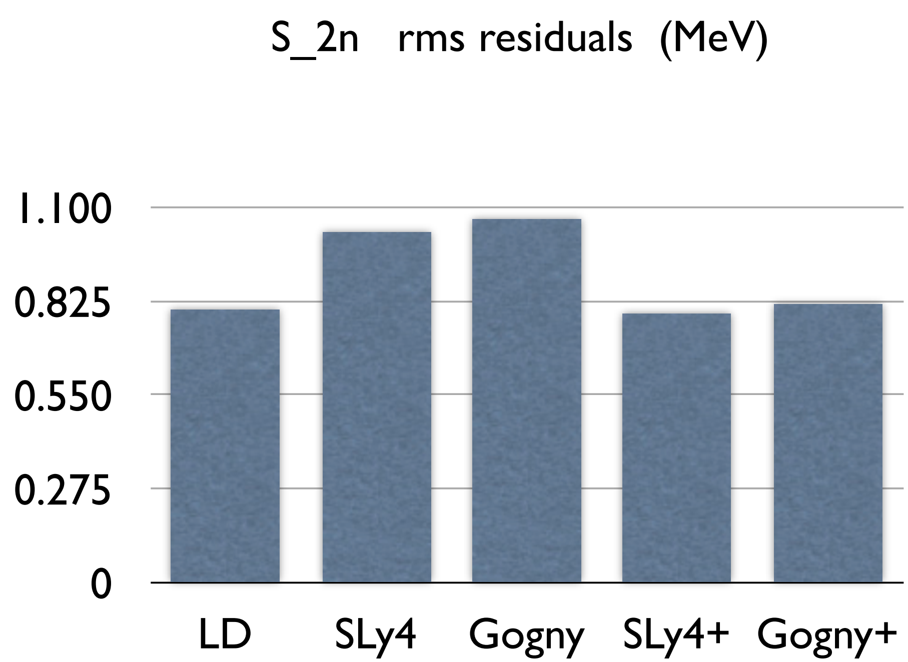
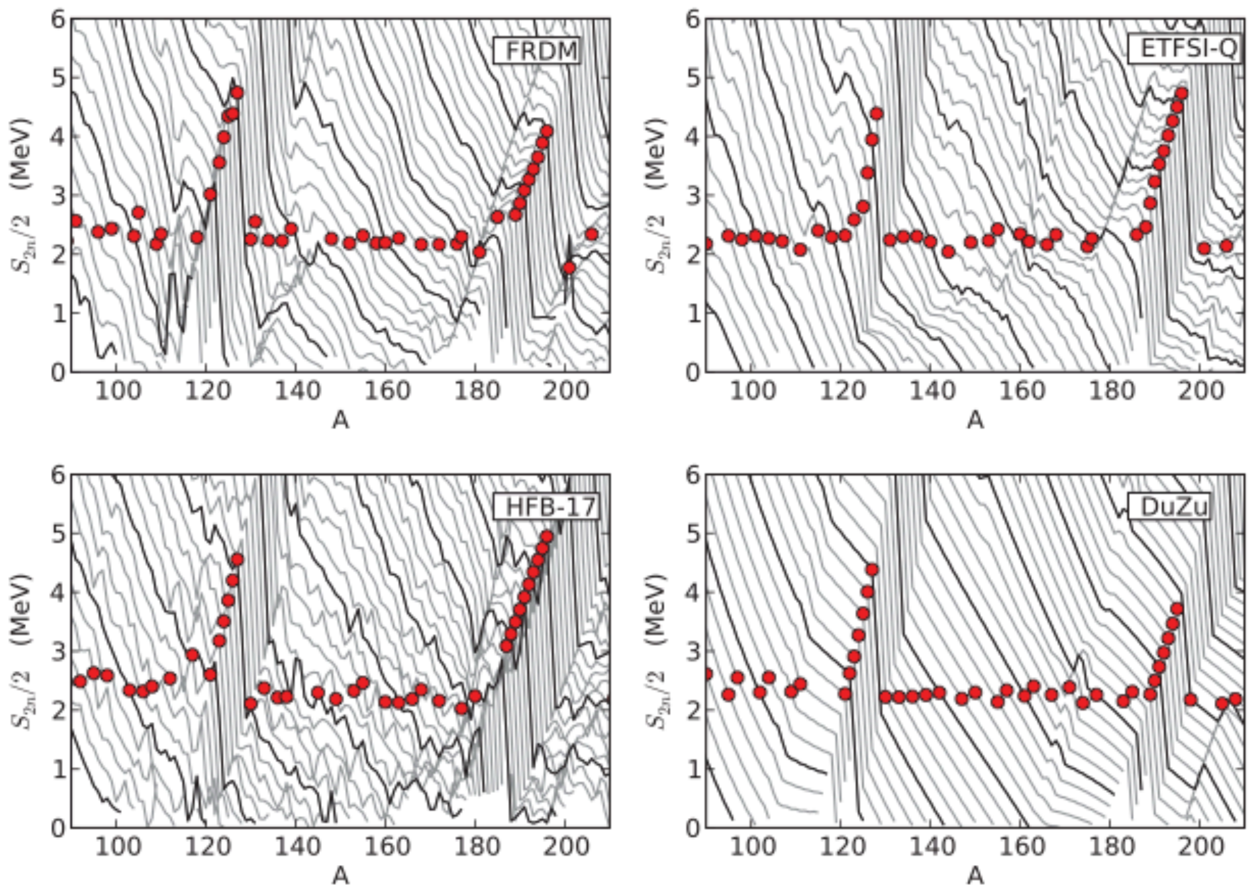


FIG. 2. Two-proton gaps, Eq. (3), for Pb and Sn isotopic chains. Theoretical curves are the following: spherical mean field (short dashed lines); mean field allowing for static deformations (long dashed lines); present theory (solid lines). Experimental values [1] are shown as diamonds.


S_2n rms residuals (MeV)
1.100
0.825
0.550
0.275
0
LD
SLy4
Gogny
SLy4+
Gogny+

r-Process nucleosynthesis

Arcones and Martinez-Pinedo, PRC83



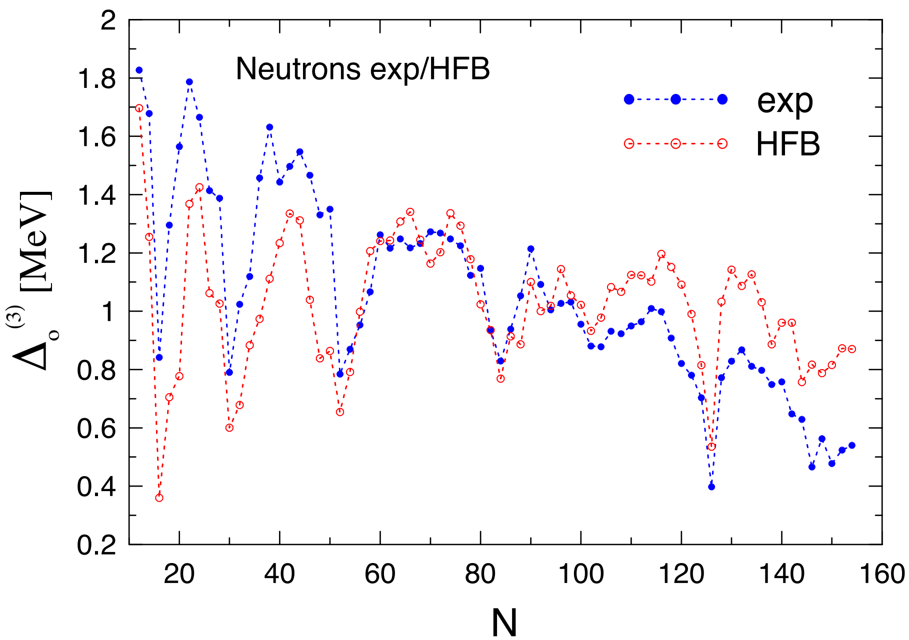
Odd-even mass staggering

aka pairing gaps

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

rms residuals for 443 nuclei (MeV)

Theory	σ	projected
Constant	0.31	
c/A^α	0.24	
HFB	0.27	0.23
HF+BCS	0.28	0.24



Phenomenology is hard to beat!