Towards a Universal Density Functional for the Nucleus
Institute for Nuclear Theory, UW Seattle, September 26-30, 2005

Going beyond the mean-field: configuration mixing of symmetry-restored mean-field states

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Self-Consistent Mean Field Models 101: Ingredients

1.) independent (quasi-) particle states

2.) effective interaction

3.) self-consistency

4.) stationary states $\Rightarrow$ equations-of-motion

- full model space of occupied states
- universal effective interaction or energy density functional
  (no agreement about a unique interaction, though: Skyrme, Gogny, Fayans, relativistic Lagrangians, . . . ; many parameterizations thereof)
- Intuitive interpretation in terms of { shapes of a nuclear liquid; shells of single-particle states }

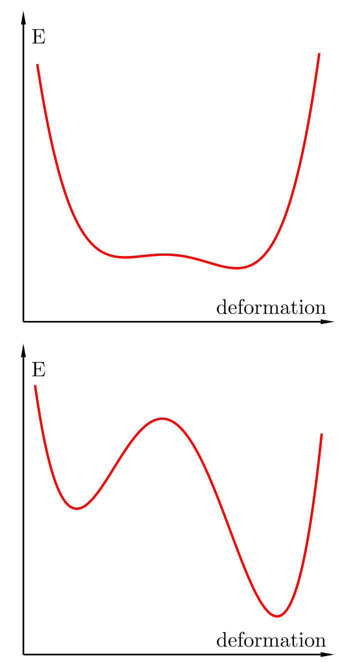
Self-Consistent Mean Field Models 101: Limitations and Problems

- very limited access to spectroscopy
  - certain rotational bands in well-deformed nuclei through cranking
  - (harmonic) vibrations from linear response theory in the small amplitude limit of time-dependent mean-field theory (QRPA); no coupling between excitation modes.
- nuclei are described in a body-fixed intrinsic frame

⇒ symmetry breaking. Mean-field states are not eigenstates of

particle number	for HFB states (pairing)
momentum	for finite nuclei
angular momentum	for deformed nuclei
parity	for octupole-deformed nuclei

⇒ done on purpose: adds np-nh and p-p shell-model correlations
⇒ but: still missing correlations related to symmetry restoration
⇒ difficult connection to the lab frame for spectroscopic observables



- arbitrary when energy changes slowly with collective coordinate: transitional nuclei ⇔ many near-degenerate mean-field states
- interpretation of coexisting minima: mean-field states with different deformation are not orthonormal.

Correlations within and beyond the mean field

Some semantics:

- static correlations: deviation of a single deformed and paired mean-field state from a spherical Slater determinant.
- dynamical correlations: fluctuations around a mean-field state, to be described by a coherent superposition of many mean-field states.

- All short-range correlations are assumed to be integrated out in the effective interaction.

Going Beyond the Mean Field I: Projection (After Variation)

- particle-number projection (separately for protons and neutrons)

$$\hat{P}_{N_0} = \frac{1}{2\pi} \int_0^{2\pi} d\phi_N \; e^{i\phi_N(\hat{N}-N_0)}$$

- angular-momentum projection

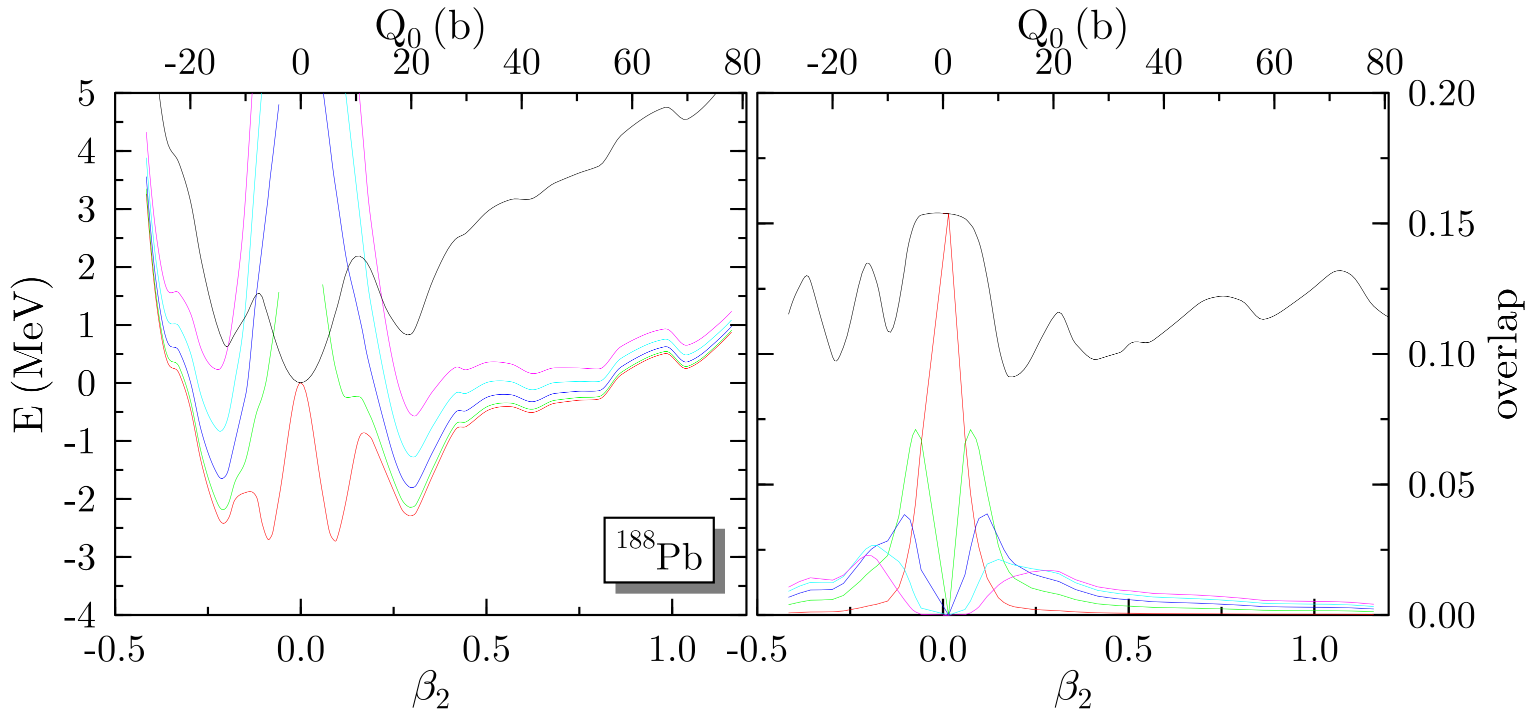
$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{4\pi} d\alpha \int_0^{\pi} d\beta \; \sin(\beta) \int_0^{2\pi} d\gamma \; \underbrace{\mathcal{D}^{*J}_{MK}(\alpha,\beta,\gamma)}_{\text{Wigner function}} \; \overbrace{\hat{R}(\alpha,\beta,\gamma)}^{\text{rotation operator}}$$

$$\underbrace{|JMN_0Z_0q\rangle}_{\text{projected state}} = \frac{1}{\mathcal{N}} \sum_{K=-J}^{+J} F^{J*}_K \; \hat{P}^J_{MK} \; \hat{P}_{N_0} \; \hat{P}_{Z_0} \quad \underbrace{|q\rangle}_{\text{mean-field state}}$$

Significantly simplified for matrix elements of axial states
— one rotation angle only, no K mixing

$$\hat{P}^J_{M0} = \frac{2J+1}{2} \int_0^{\pi} d\beta \; \sin(\beta) \; d^J_{M0}(\beta) \; \hat{R}(0,\beta,0)$$

Going Beyond the Mean Field I: Projection (After Variation)



Going Beyond the Mean Field II: Configuration Mixing via the Generator Coordinate Method

mixed projected many-body state: $|JMi\rangle = \sum_q f_{Ji}(q)\,|JMq\rangle$ $\left\{ \begin{array}{ll} f_{Ji}(q) & \text{weight function} \\ |JMq\rangle & \text{projected mean-field state} \end{array} \right.$

stationarity: $\frac{\delta}{\delta f^*_{Ji}(q)} \frac{\langle JMi|\hat{H}|JMi\rangle}{\langle JMi|JMi\rangle} = 0$

⇒ Hill-Wheeler-Griffin equation

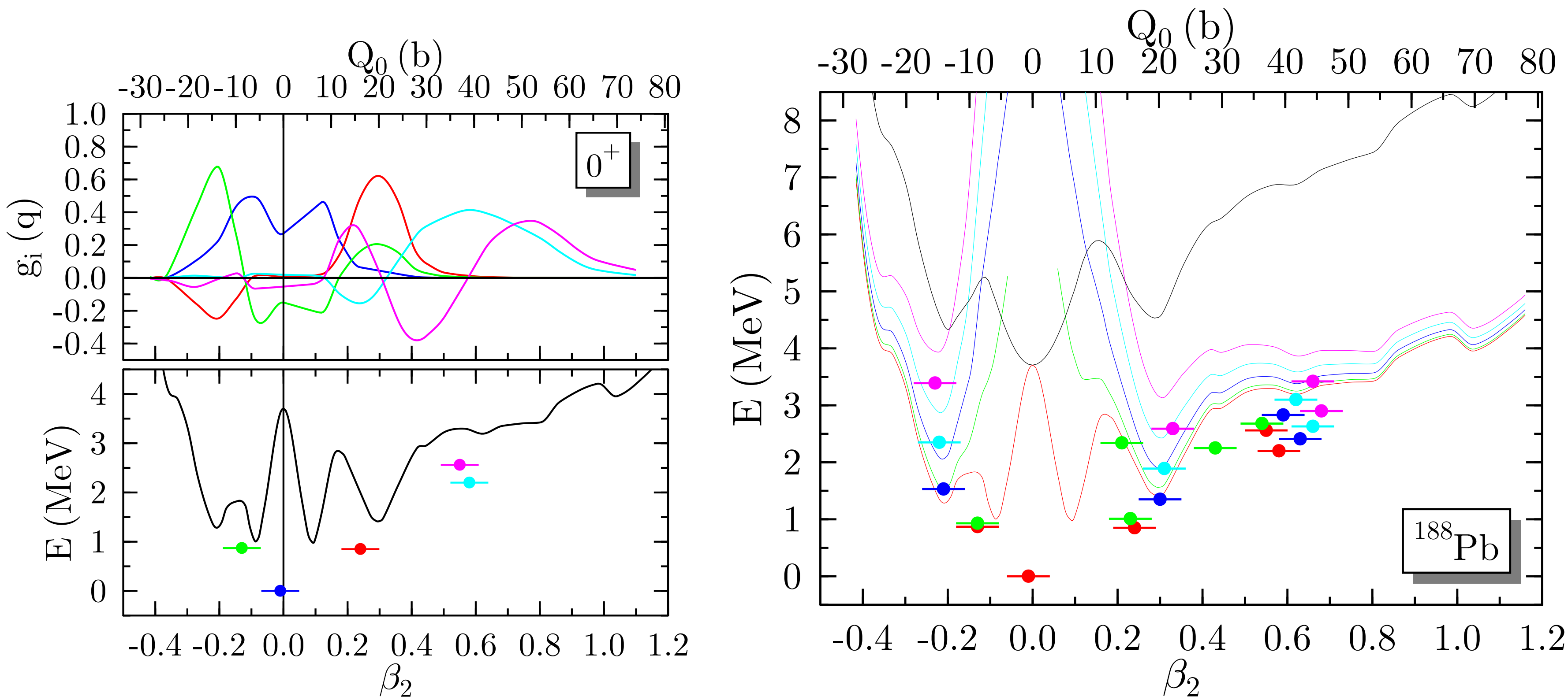
$$\sum_{q'} \left[\mathcal{H}_J(q,q') - E_i\,\mathcal{I}_J(q,q')\right] f_{J,i}(q') = 0 \qquad \left\{ \begin{array}{lll} \mathcal{H}_J(q,q') = \langle JMq|\hat{H}|JMq'\rangle & \text{Hamiltonian kernel} \\ \mathcal{I}_J(q,q') = \langle JMq|JMq'\rangle & \text{norm kernel} \end{array} \right.$$

- correlated ground state (for each J)
- excited states (from orthogonalisation to the ground state)
- the weight functions $f^J_k(q)$ are not orthonormal

⇒ orthonormal collective wave functions are obtained as $g_k(q) = \sum_{q'} \mathcal{I}^{1/2}(q,q')\,f_k(q')$

D. L. Hill, J. A. Wheeler, Phys. Rev. **89** (1953) 1102; J. J. Griffin, J. A. Wheeler, *ibid.* **108** (1957) 311

Going Beyond the Mean Field II: Configuration Mixing via the Generator Coordinate Method



M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.

Going Beyond the Mean Field II: Configuration Mixing via the Generator Coordinate Method

• Projection is a special case of the GCM, where exactly degenerated states are mixed. The generators of the symmetry group involved define the collective path, while the weight function is determined by the restored symmetry.

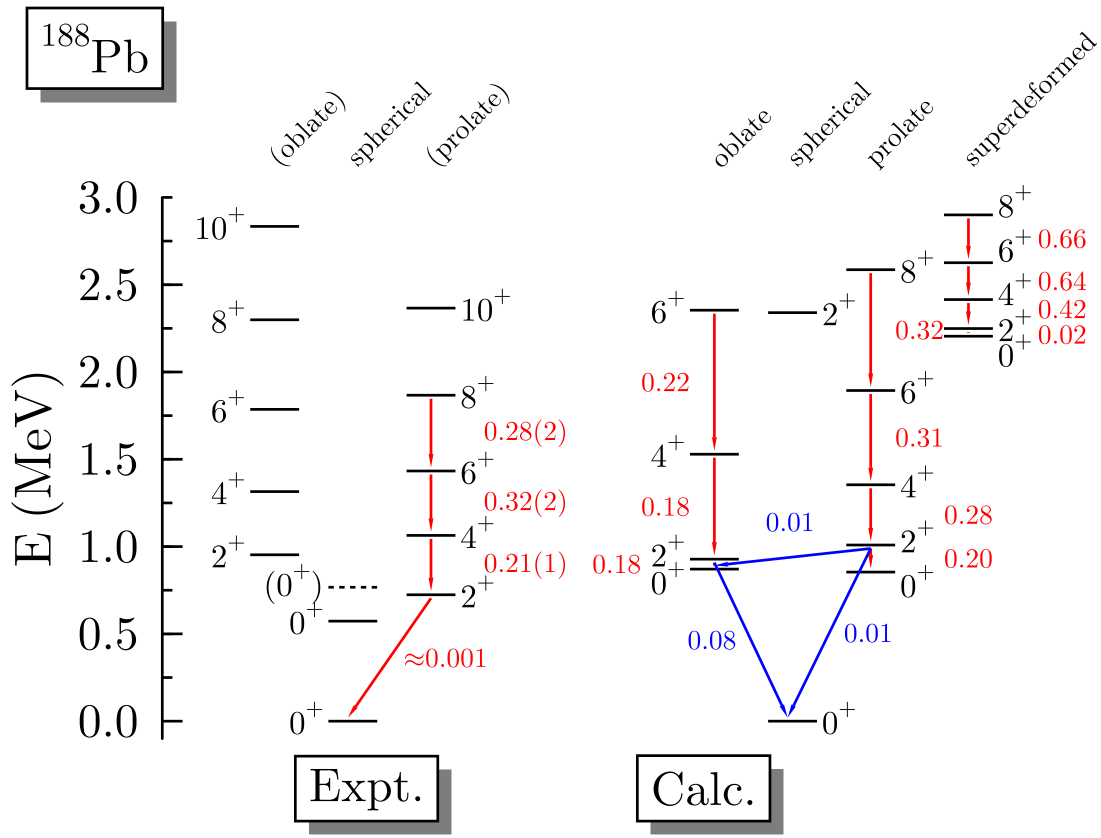
• Angular momentum-projection is part of what can be called "quadrupole correlations", as it mixes states with different orientations of the quadrupole tensor.

$\Rightarrow$ For consistency, configuration mixing of states with different quadrupole moment should be done together with angular momentum projection.

• There is no collective potential or collective mass in the GCM method – they appear in approximations to the GCM as, for example, the Bohr-Hamiltonian.

• Without exact particle-number projection, it is not guaranteed that matrix elements between different mean-field states have the right particle number. Projection eliminates the problem, otherwise one has to use correction schemes that add further approximations.

• There is conservation of trouble: by introducing spurious divergencies, particle-number projection causes new problems that one does not have without (see Mario Stoitsov's talk)



$$\beta_2^{(t)}(J_k) = \frac{4\pi}{3R^2A}\sqrt{\frac{B(E2;J_k\to J'_k-2)}{\langle J\,0\,2\,0|(J-2)\,0\rangle^2 e^2}} \quad \text{with} \quad R=1.2\,A^{1/3}$$

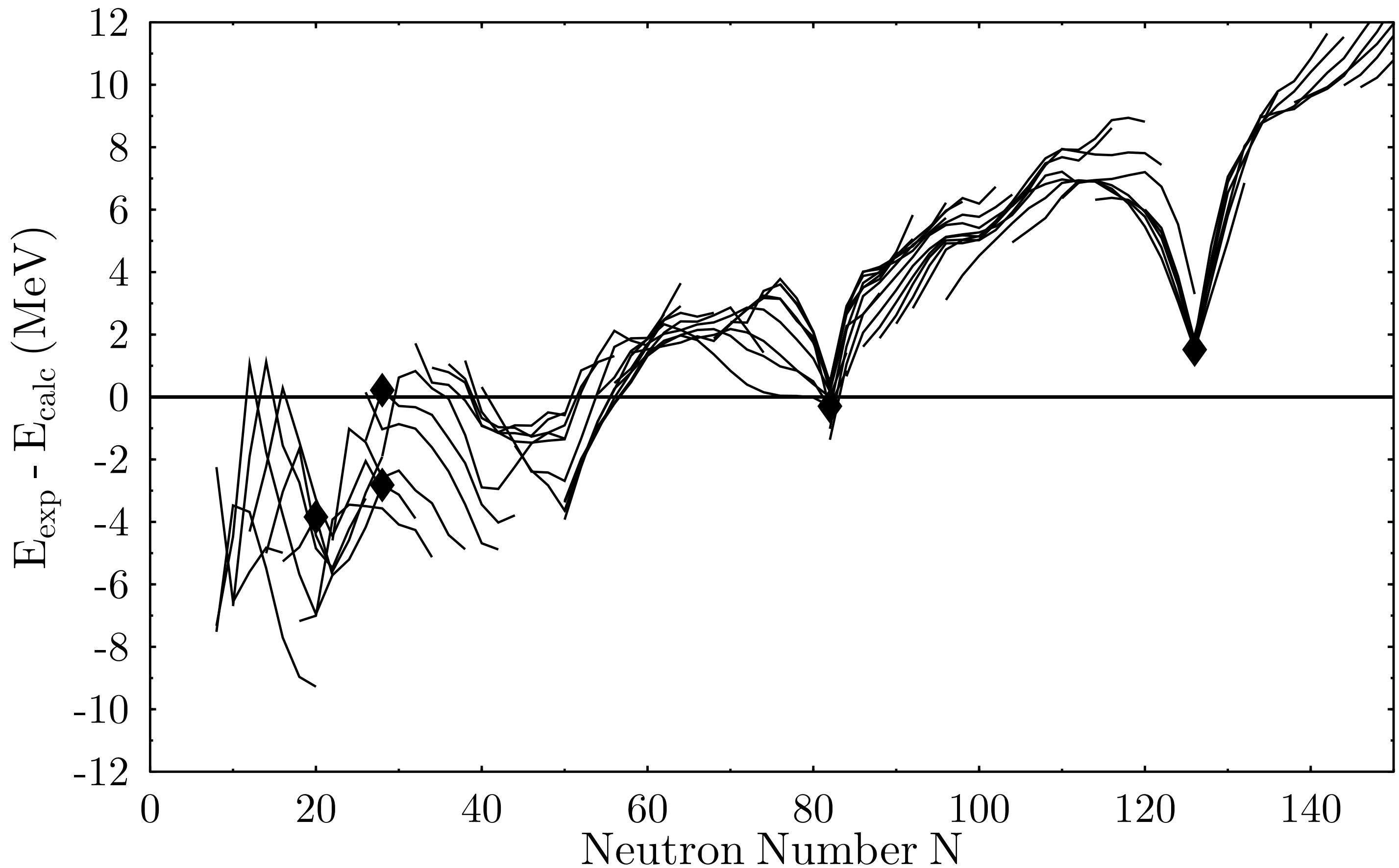
$$B(E2;J'_{k'}\to J_k) = \frac{e^2}{2J'+1}\sum_{M=-J}^{+J}\sum_{M'=-J'}^{+J'}\sum_{\mu=-2}^{+2}|\langle JMk|\hat{Q}_{2\mu}|J'M'k'\rangle|^2 = \frac{e^2}{2J'+1}\Big|\sum_{q,q'} f^*_{J,k}(q)\, f_{J',k'}(q')\,\langle Jq||\hat{Q}_2||J'q'\rangle\Big|^2$$

Promesse: Mixing of axially symmetric time-reversal-invariant states

- configuration mixing of particle-number and angular-momentum projected states
- mass quadrupole moment serves as the generator coordinate
- time-reversal invariant self-consistent HF+BCS or HFB states
- full model space of occupied particles.
- approximate particle-number projection before variation à la Lipkin-Nogami
- representation of the single-particle states on a 3d Lagrange mesh
- restriction to axially and reflection-symmetric shapes $\Rightarrow$ J even, $K = 0$, $P = +1$
- Skyrme interaction SLy4 or SLy6 in the particle-hole channel
  + density-dependent local pairing interaction (“surface pairing”)

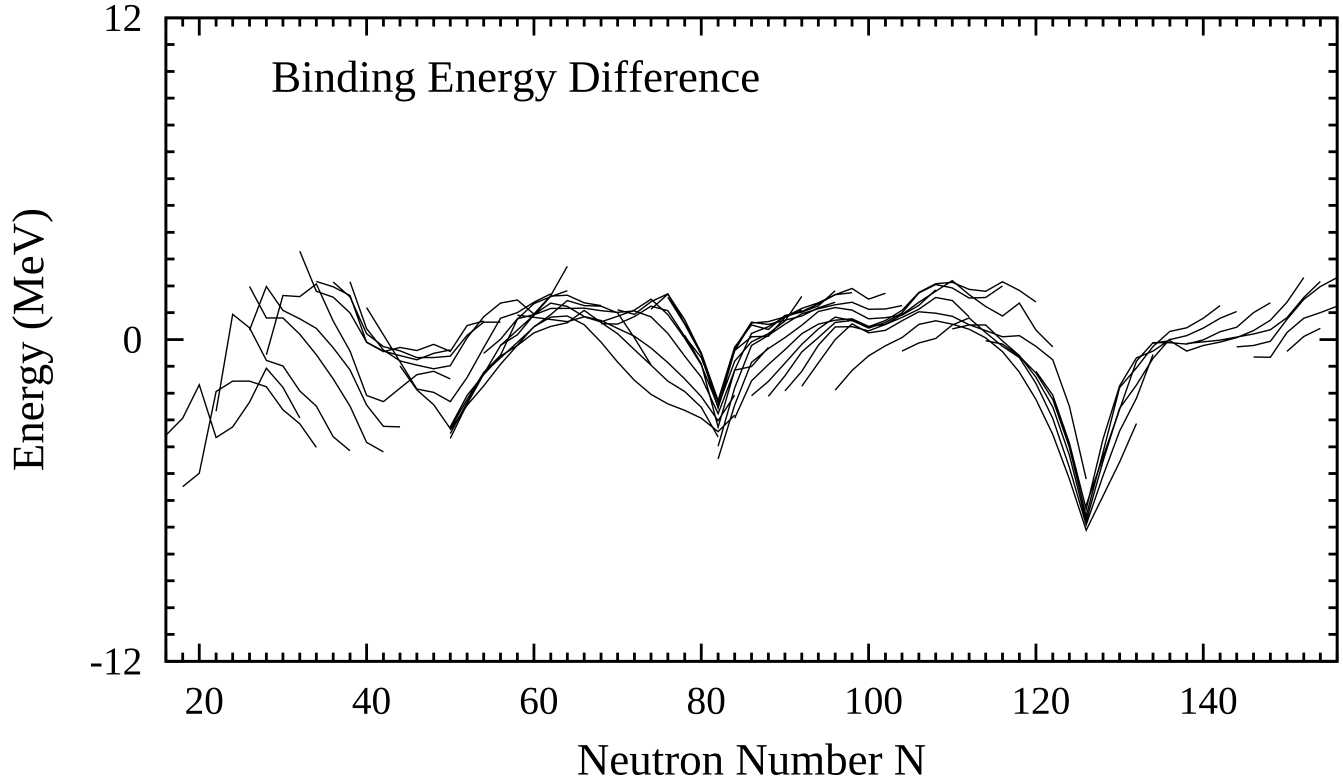
^{24}Mg	A. Valor, P.-H. Heenen, P. Bonche, Nucl. Phys. A671 (2000) 145.
^{16}O	M. B., P.-H. Heenen, Nucl. Phys. A713 (2003) 390.
^{32}S, ^{36,38}Ar, ^{40}Ca	M. B., H. Flocard, P.-H. Heenen, Phys. Rev. C 68 (2003) 044321.
^{186}Pb	T. Duguet, M. B., P. Bonche, P.-H. Heenen, Phys. Lett. B559 (2003) 201.
$^{182-194}$Pb	M. B., P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303.
^{240}Pu	M. B., P.-H. Heenen, P. Bonche, Phys. Rev. C 70 (2004) 054304.
correlation energies	M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C **69** (2004) 034340.
	M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503.
	M. B., G. F. Bertsch, P.-H. Heenen, nucl-th/0508052

Masses from Mean-Field Calculations



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503.

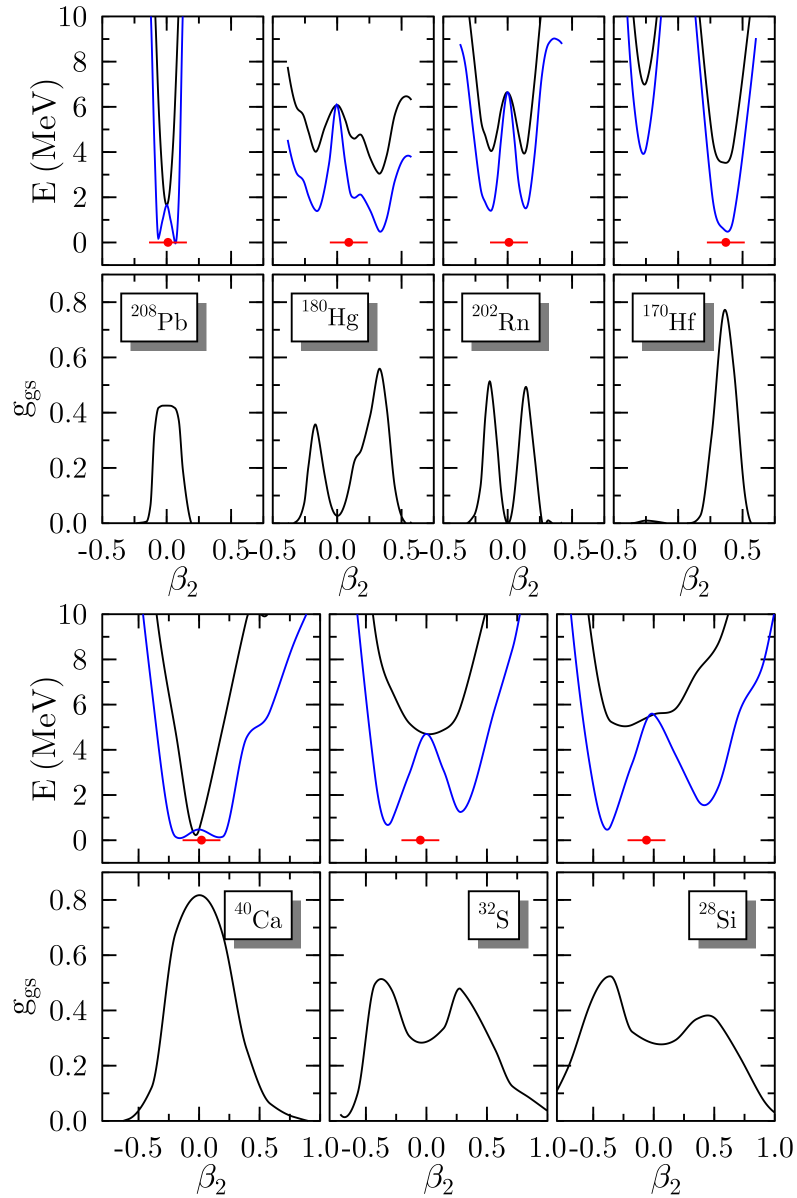
Readjustment of the density functional



- The slightly wrong trend with mass and isospin can be removed by a slight (a few permille) readjustment of the parameters of SLy4.

G. F. Bertsch, B. Sabbey, M. Uusnäkki, Phys. Rev. C 71 (2005) 054311.

Typical Situations



nucleus	E_{def}	$E_{J=0}$	E_{GCM}	E_{corr}
^{208}Pb	0.0	1.7	0.0	1.7
^{180}Hg	3.0	2.6	0.5	3.1
^{170}Hf	12.2	2.9	0.5	3.4
^{202}Rn	2.6	2.7	1.4	4.0
^{48}Ca	0.0	1.4	0.7	2.0
^{32}S	0.0	3.8	0.9	4.7
^{28}Si	0.7	4.2	0.6	4.9

M. B., G. F. Bertsch, P.-H. Heenen, nucl-th/0508052

Ground-state correlation energies made simple

- Full calculation requires

$$\left.\begin{array}{l} n_J \approx 5\ldots 15 \text{ rotated states} \\ n_q \approx 7\ldots 25 \text{ deformations} \end{array}\right\} \Rightarrow \quad n_J \times \frac{n_q(n_q+1)}{2} \approx 150\ldots 5000 \text{ mixed configurations}$$

- For large-scale calculations of masses and other ground state observables, it is desirable to have a faster method

⇒ Gaussian overlap approximation (GOA)

- topological GOA for the angular momentum projection. The rotational operator has to be applied only once

- only diagonal matrix elements and matrix elements between nearest neighbors are calculated explicitely for the GCM

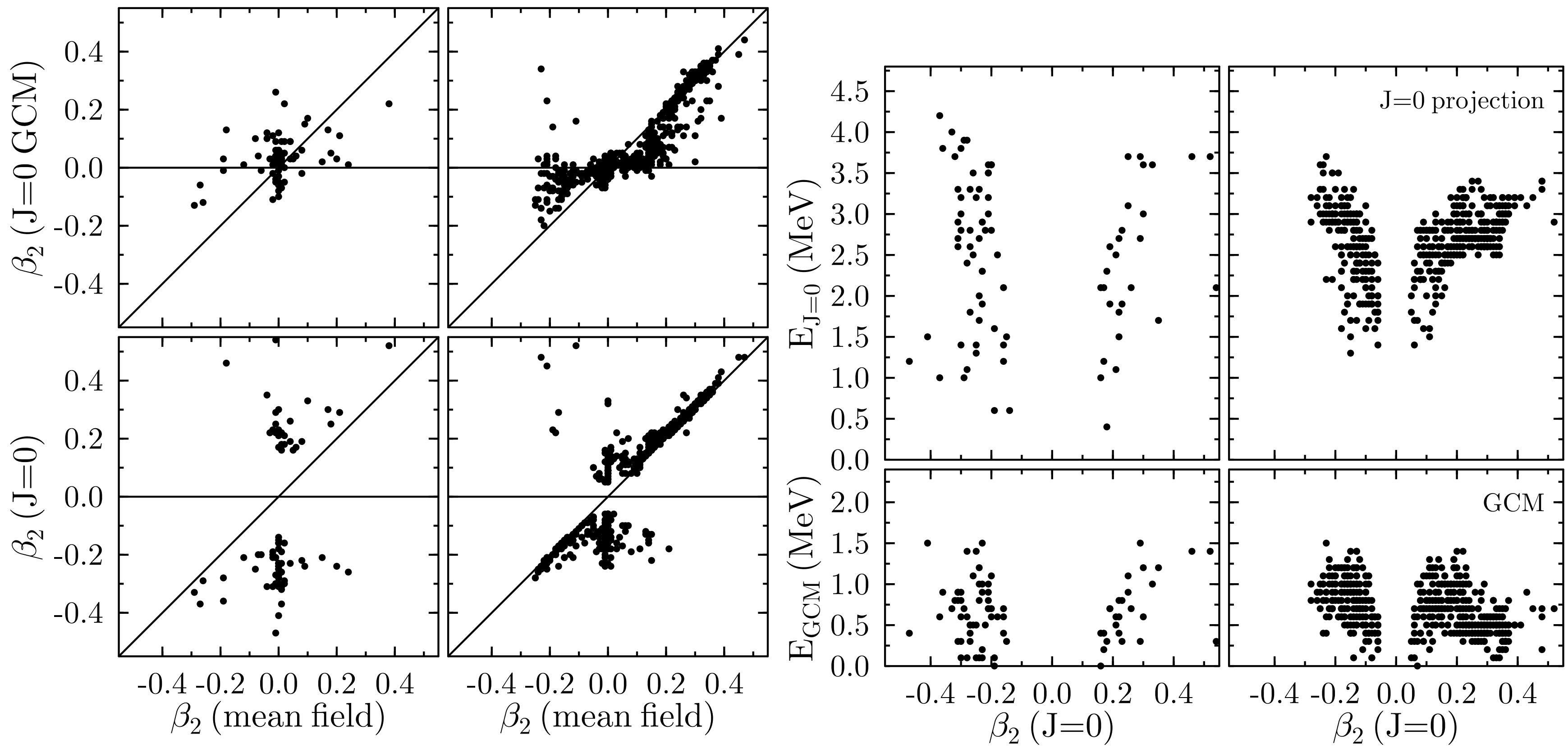
⇒ $n_J \times [n_q + (n_q - 1)] \approx 26\ldots 100$ calculated matrix elements

⇒ Accuracy better than 300 keV ⇒ sufficient for study of systematics of quadrupole correlation energies

⇒ emphasis on ground state — most information on spectroscopy is lost

M. B., G. F. Bertsch and P.-H. Heenen, Phys. Rev. C 69 (2004) 034340

Induced Deformations



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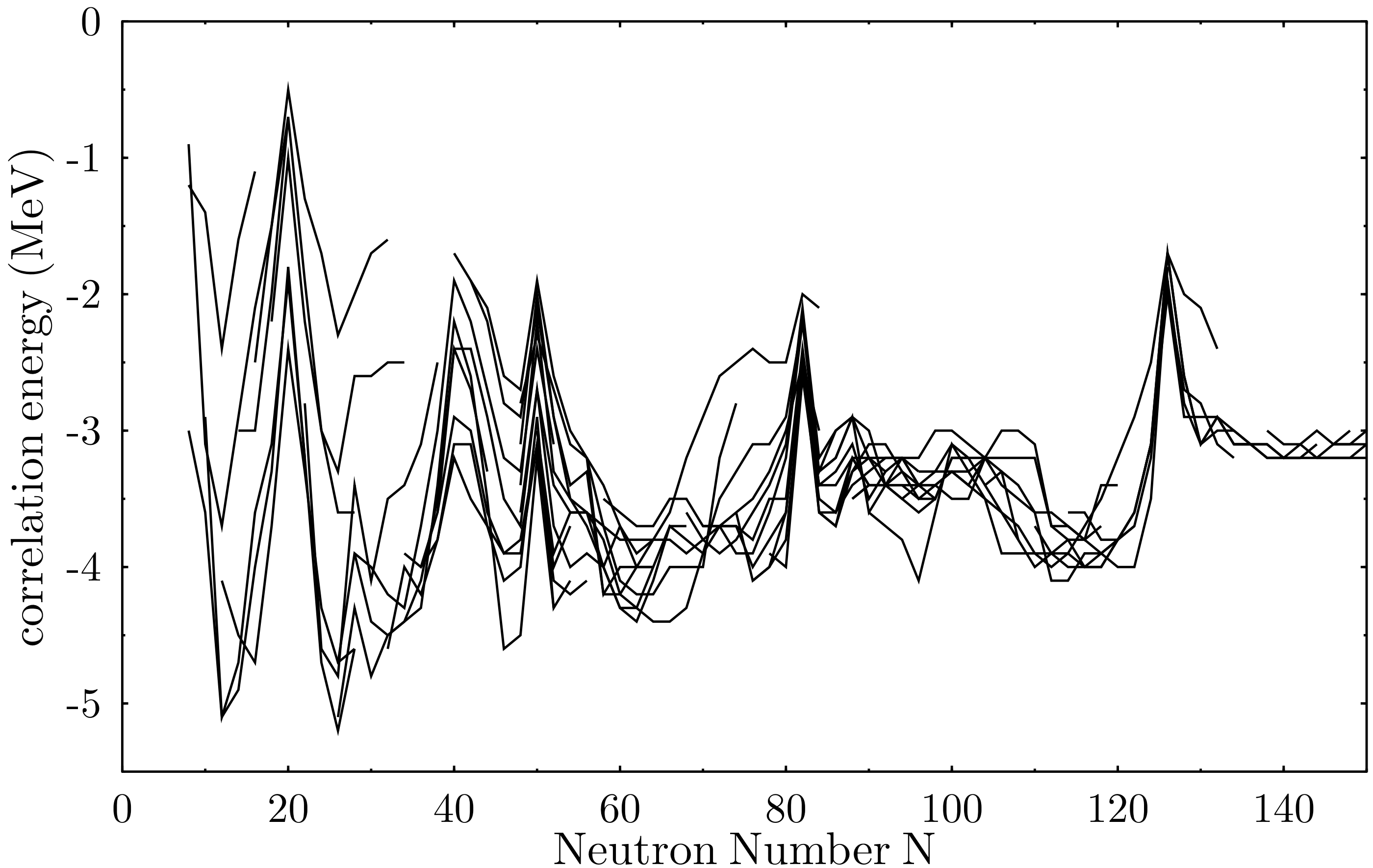
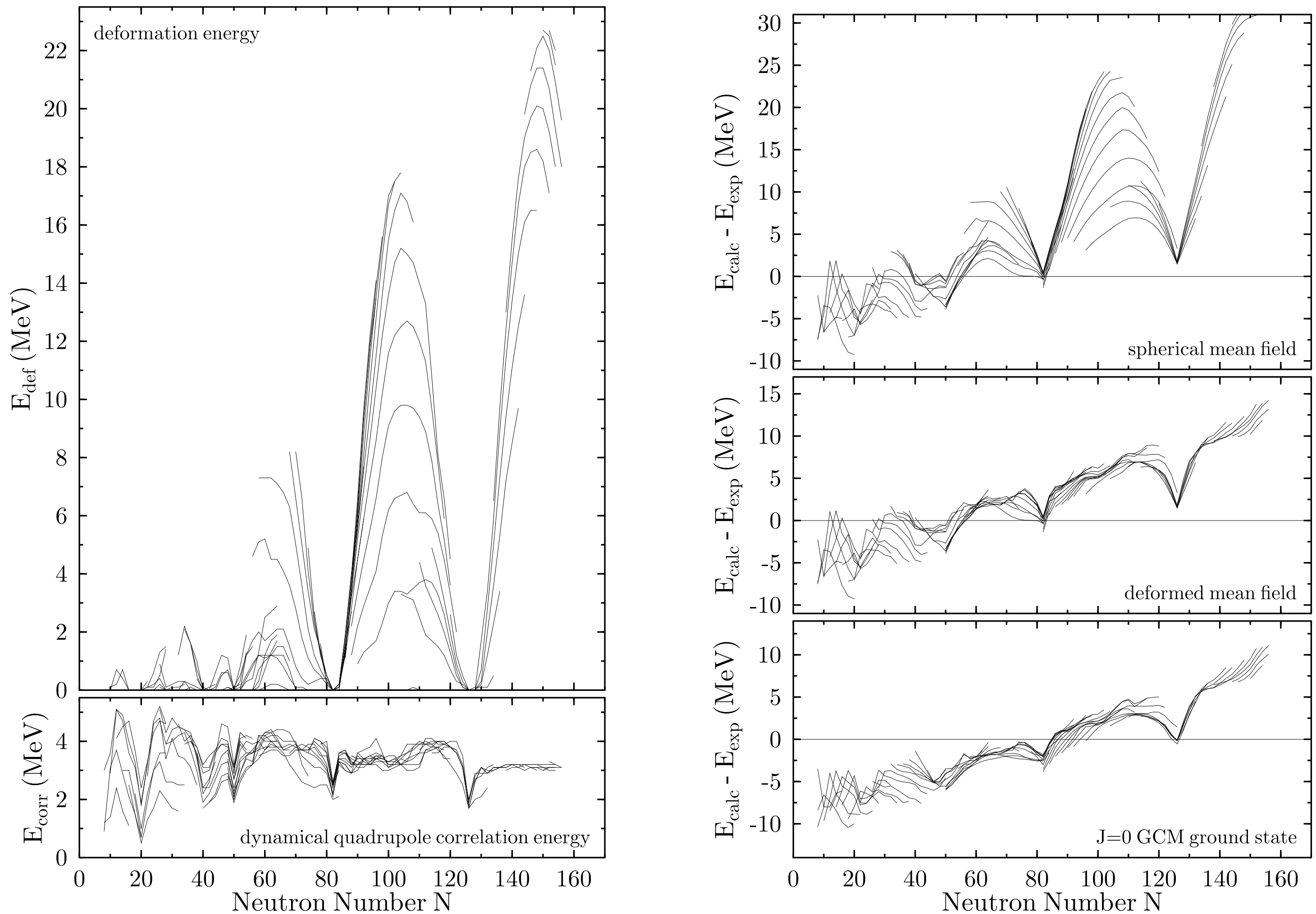
Quadrupole Correlation Energies



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503.

Static and Dynamic Quadrupole Correlation Energies



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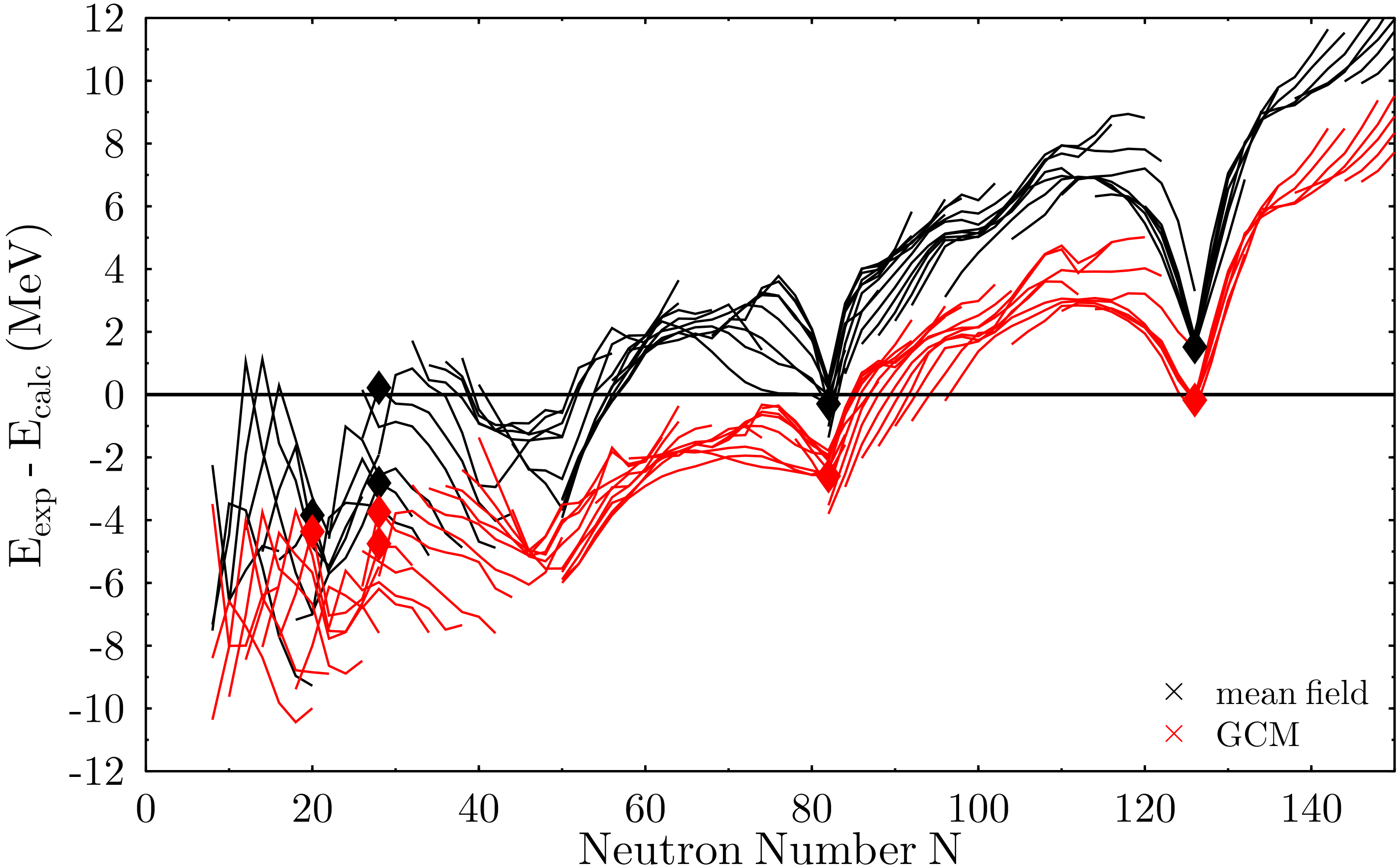
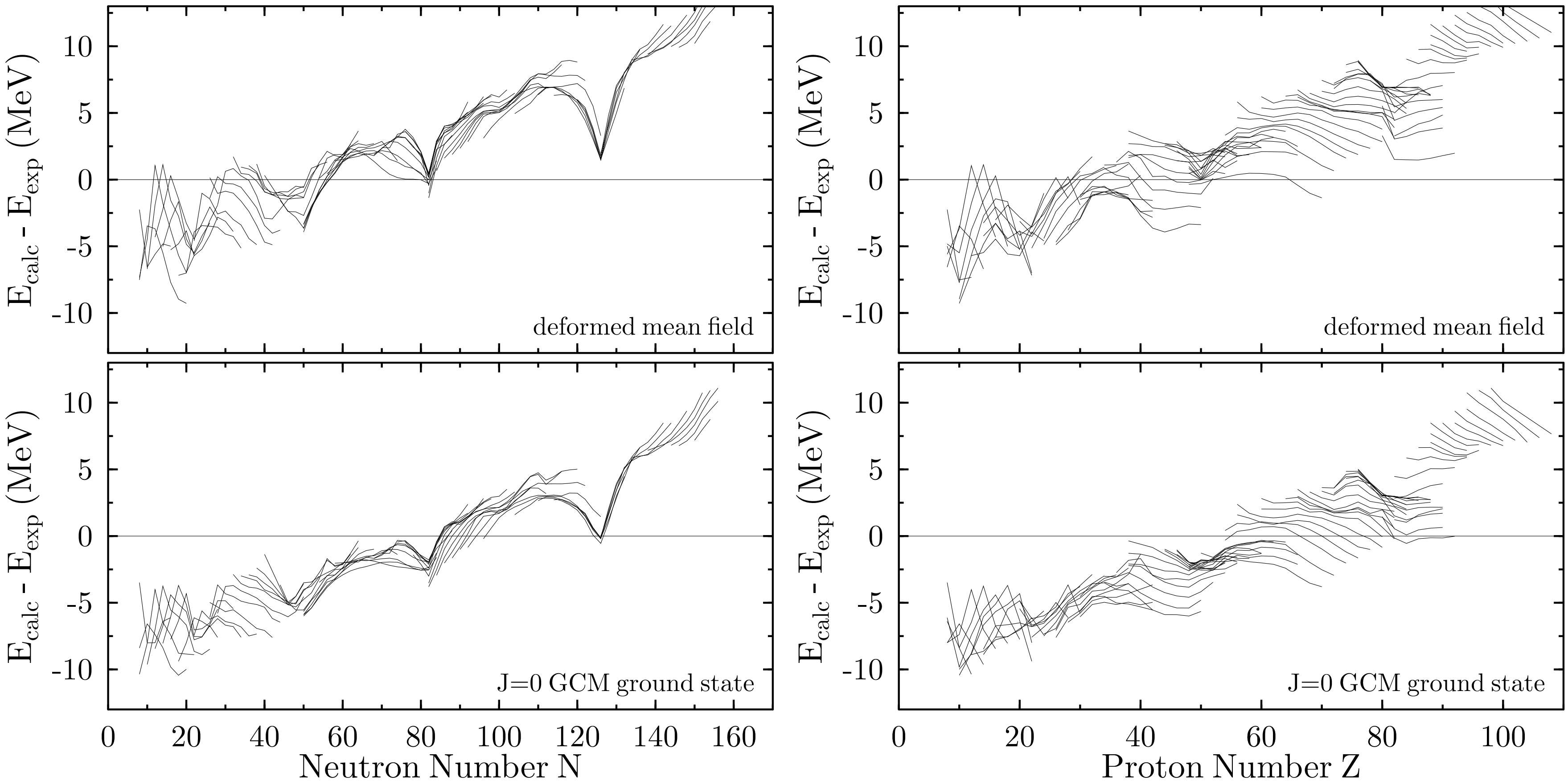
Masses including Quadrupole Correlation Energies



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503.



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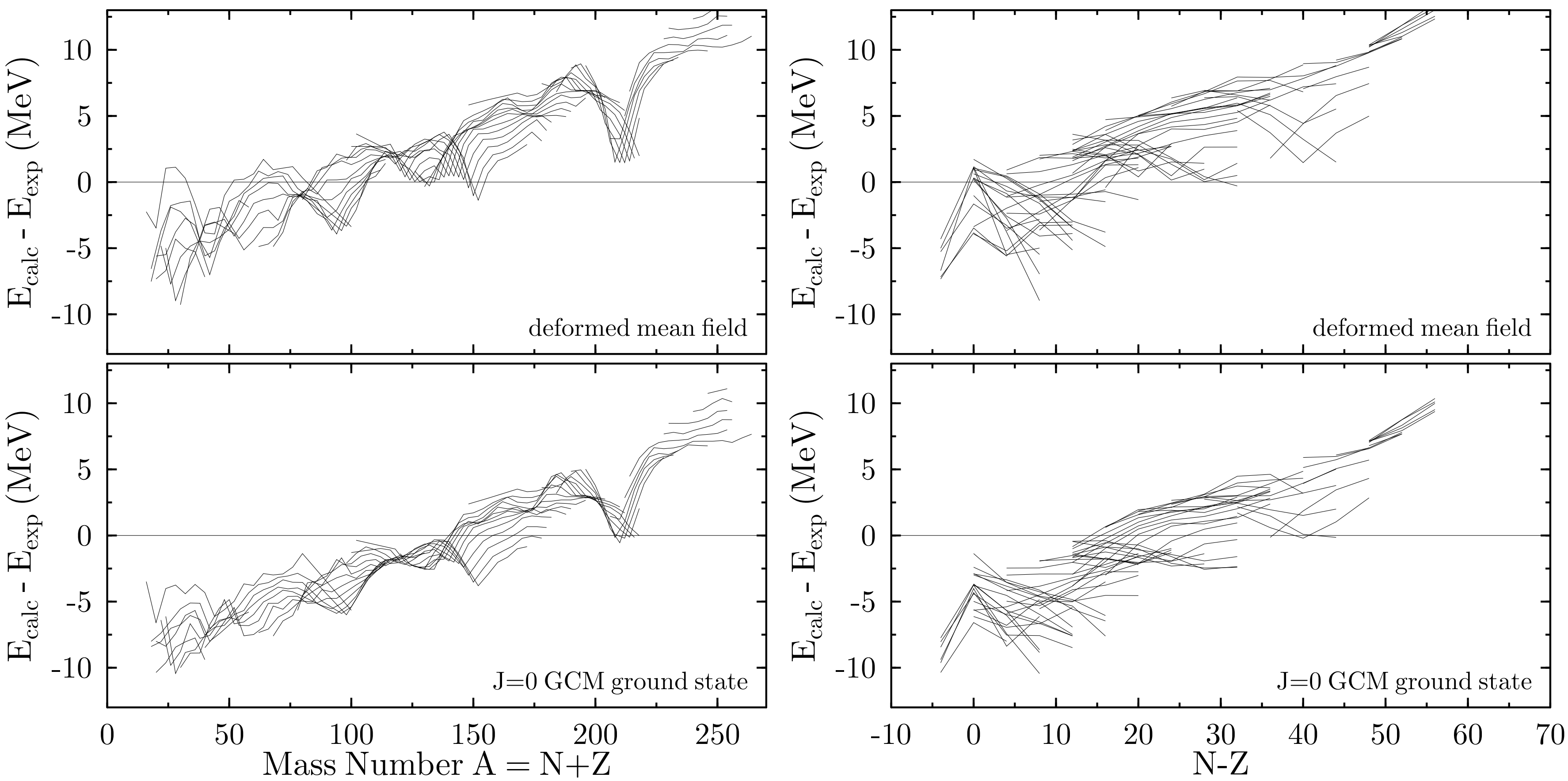

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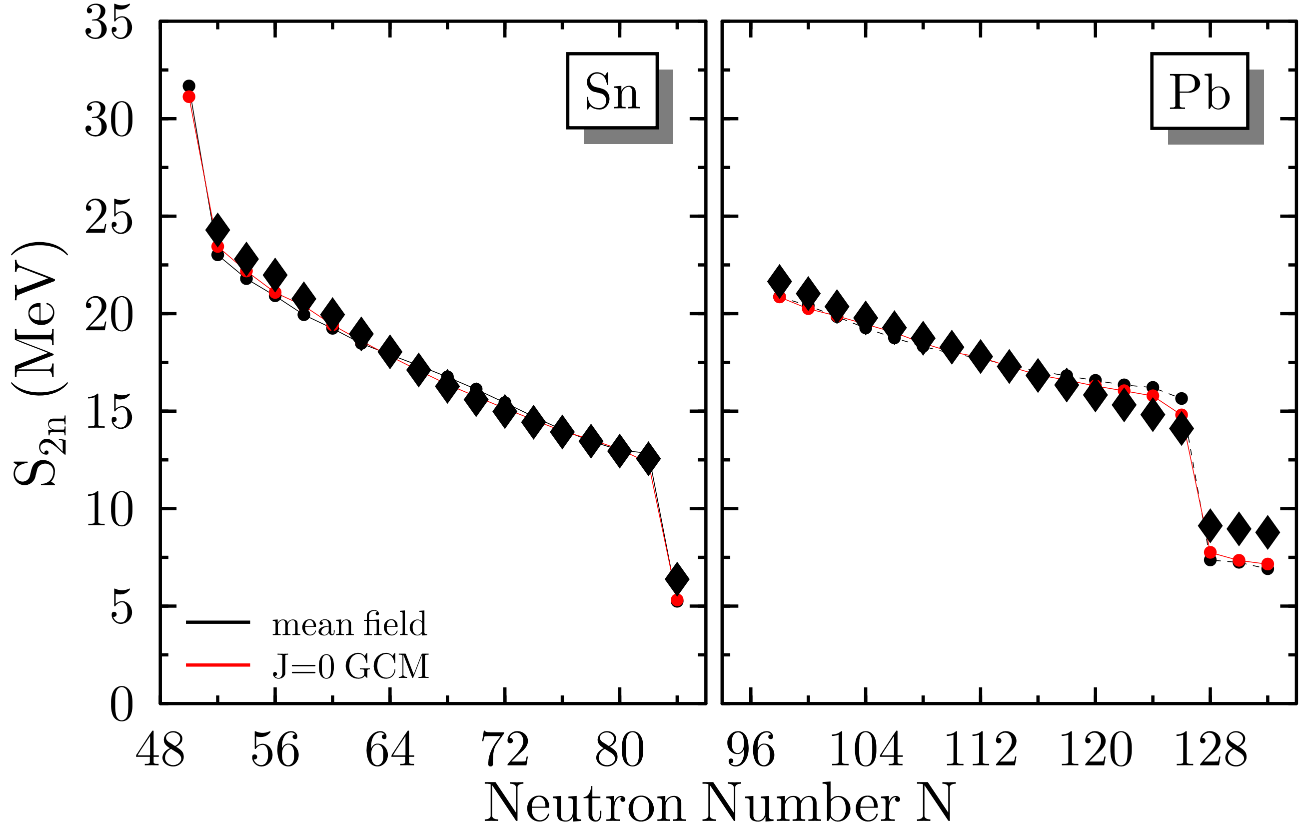
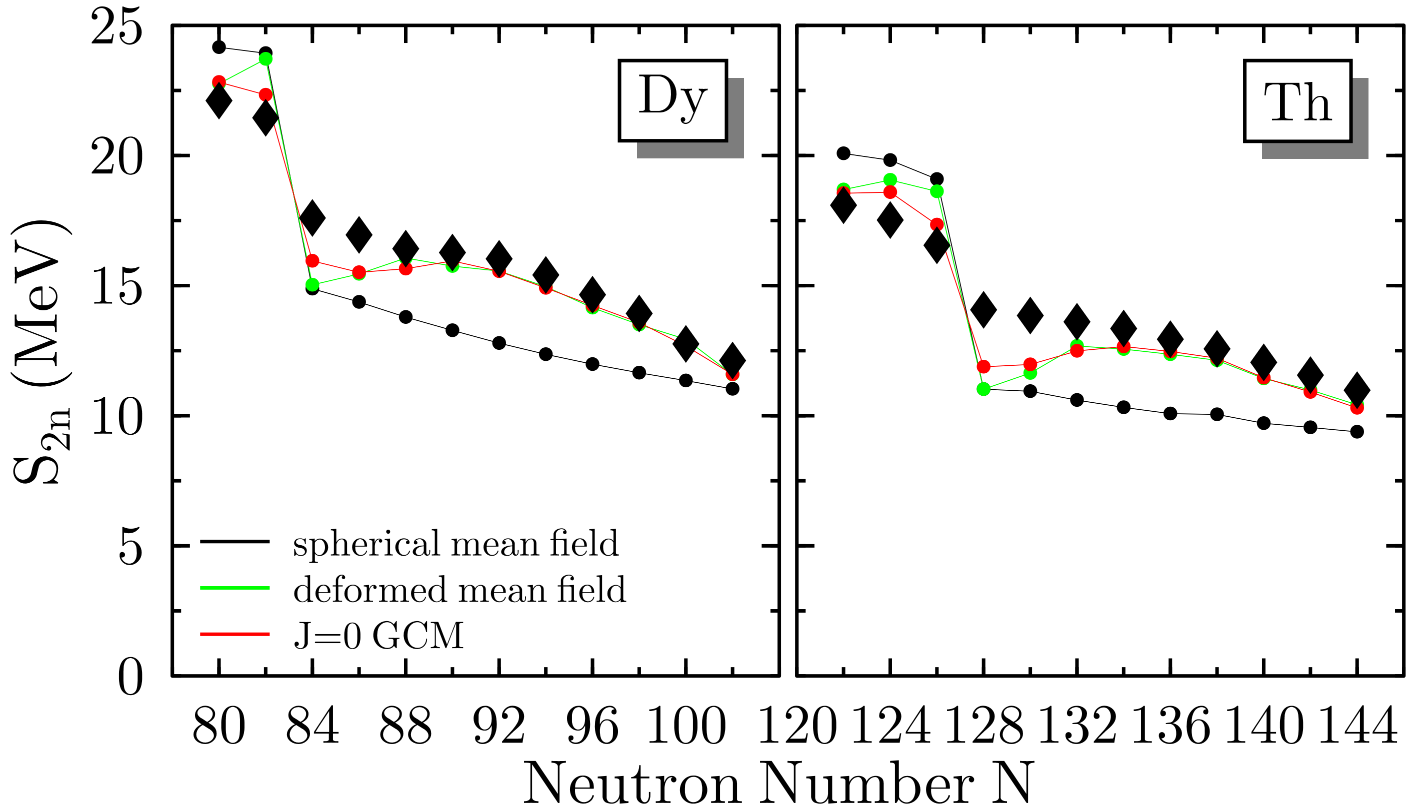
Systematics of Mass-Difference Formulas



$$S_{2n}(N,Z) = E(N-2,Z) - E(N,Z)$$

M. B., G. F. Bertsch, P.-H. Heenen, nucl-th/0508052

Systematics of Mass-Difference Formulas



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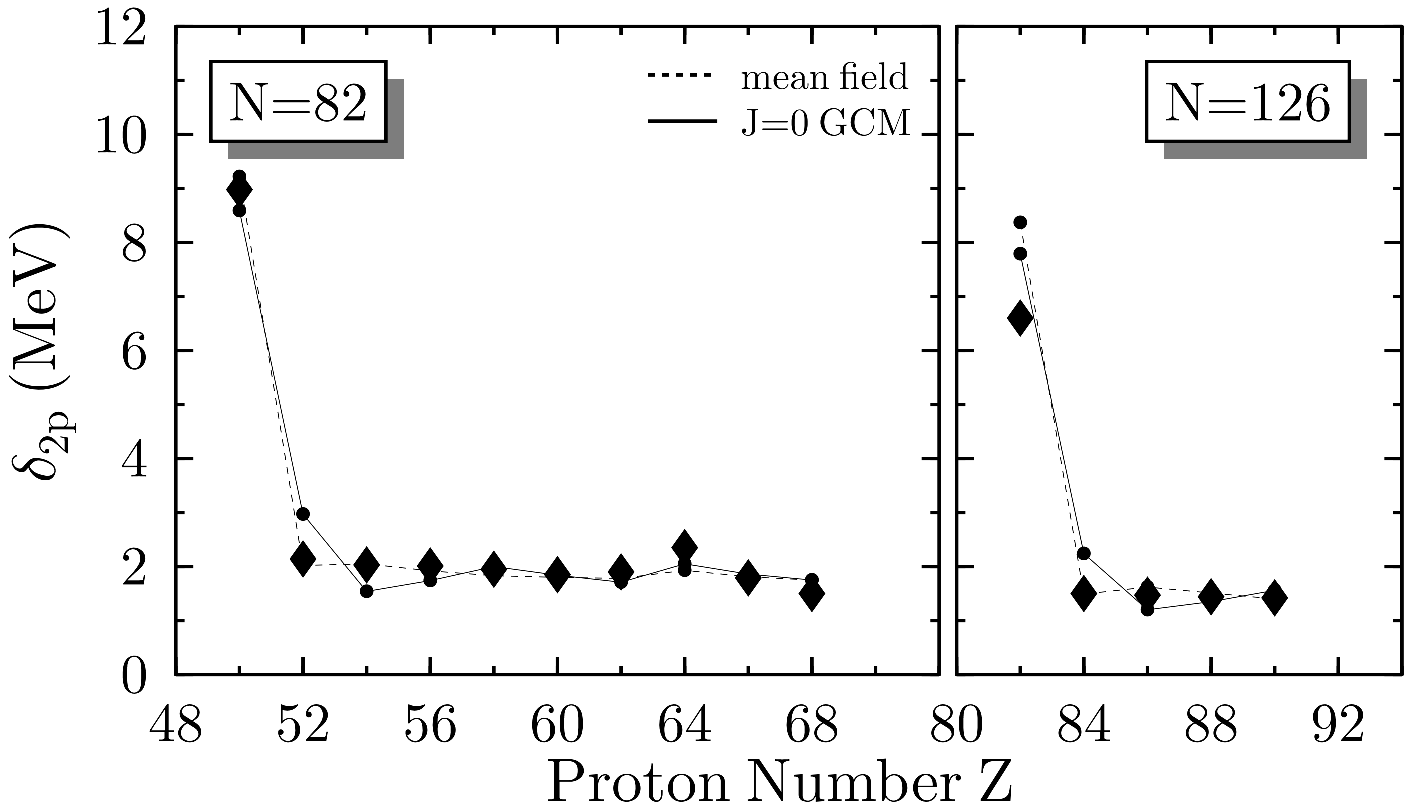

$$\delta_{2p}(N, Z) = E(N, Z-2) - 2E(N, Z) + E(N, Z+2)$$

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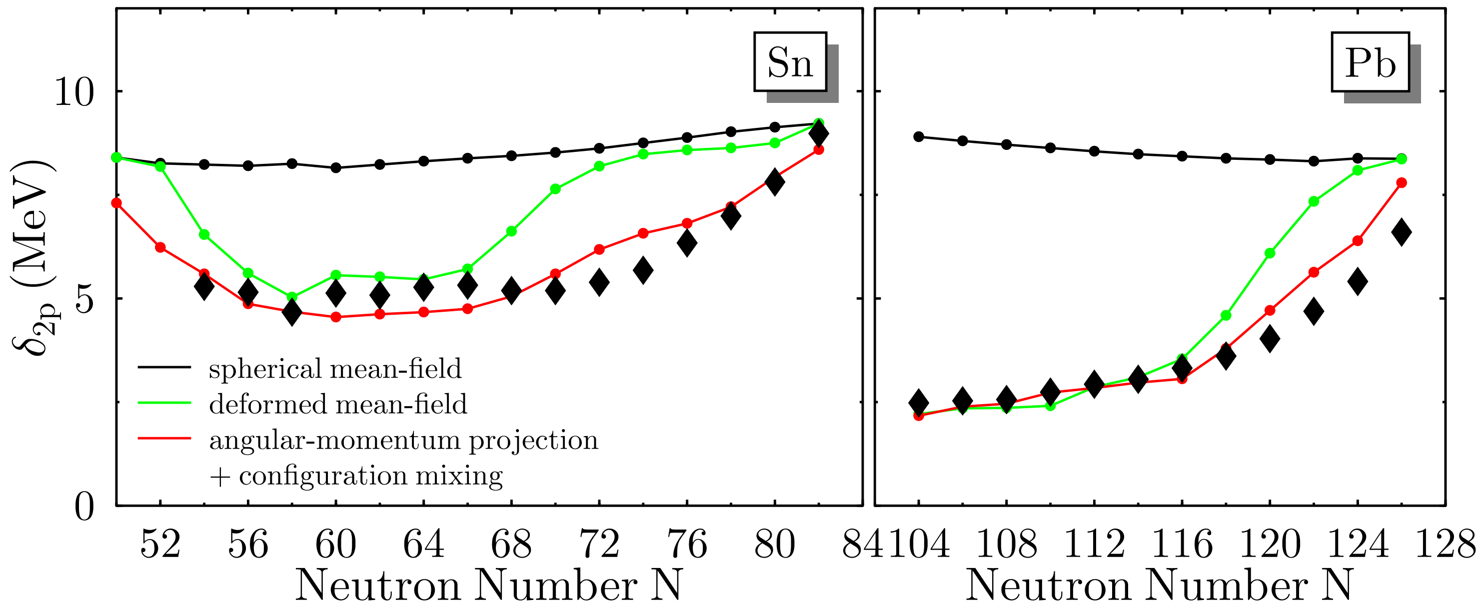
Systematics of Mass-Difference Formulas



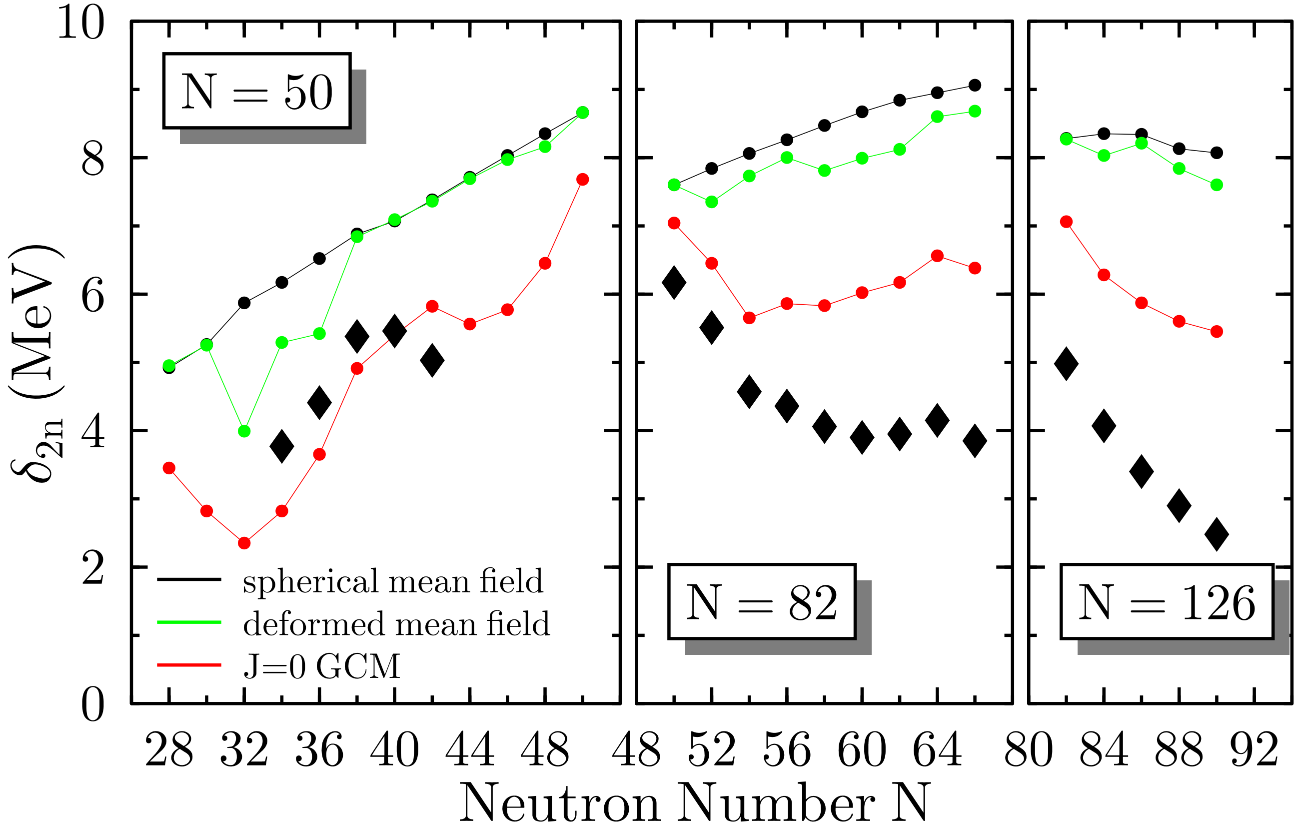
$$\delta_{2p}(N, Z) = E(N, Z-2) - 2E(N, Z) + E(N, Z+2)$$

provides an approximation to twice the gap in the single-particle spectrum at shell closures
if the intrinsic structure of the nuclei involved does not change

- This assumption is not valid for the $Z = 50$ and $Z = 82$ shells. Adjacent nuclei are much softer than the $Z = 50$ and $Z = 82$ isotopes, or even deformed.

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102505

Systematics of Mass-Difference Formulas



$$\delta_{2n}(N,Z) = E(N-2,Z) - 2E(N,Z) + E(N+2,Z)$$

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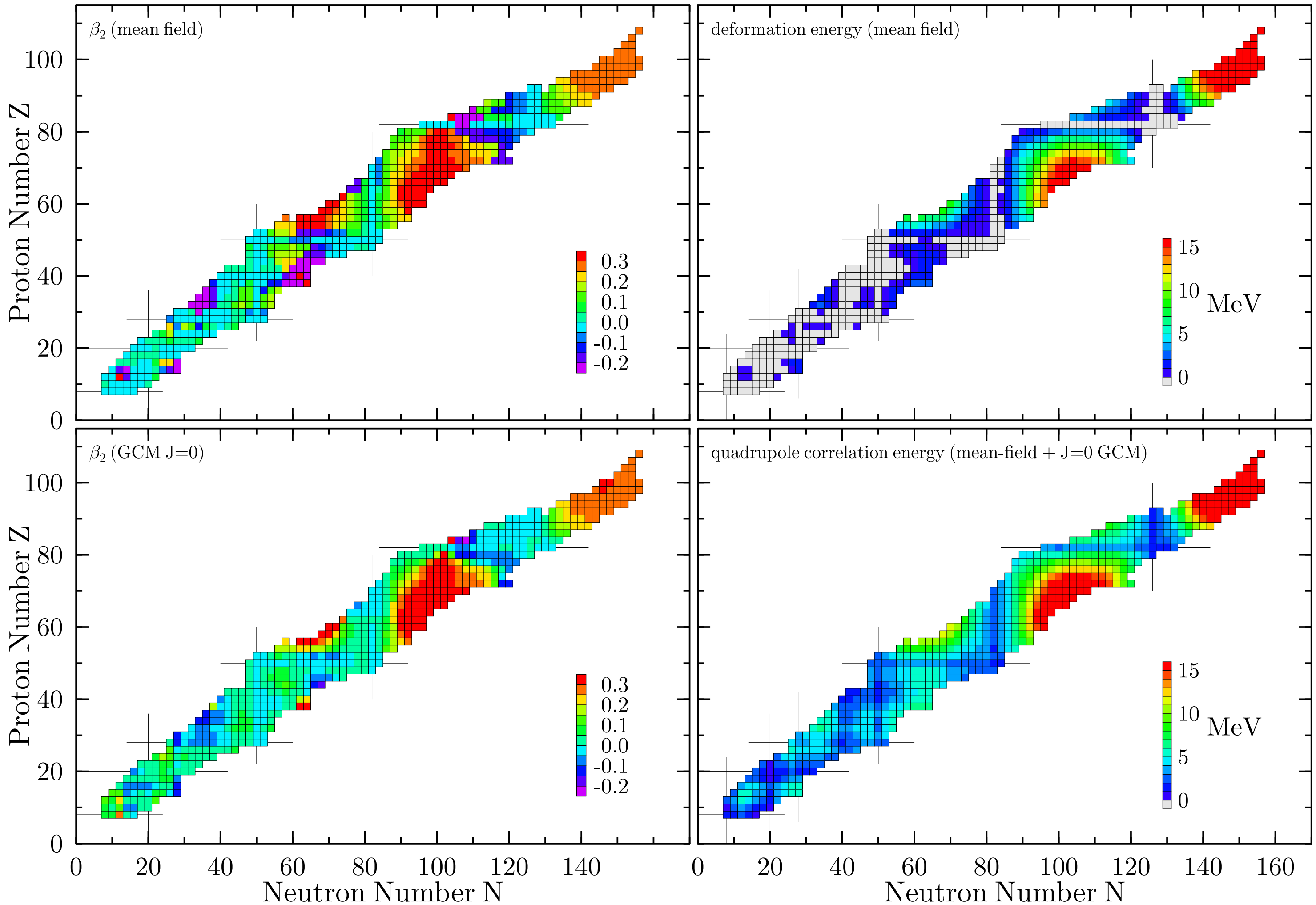
Intrinsic Deformation and Quadrupole Correlation Energy



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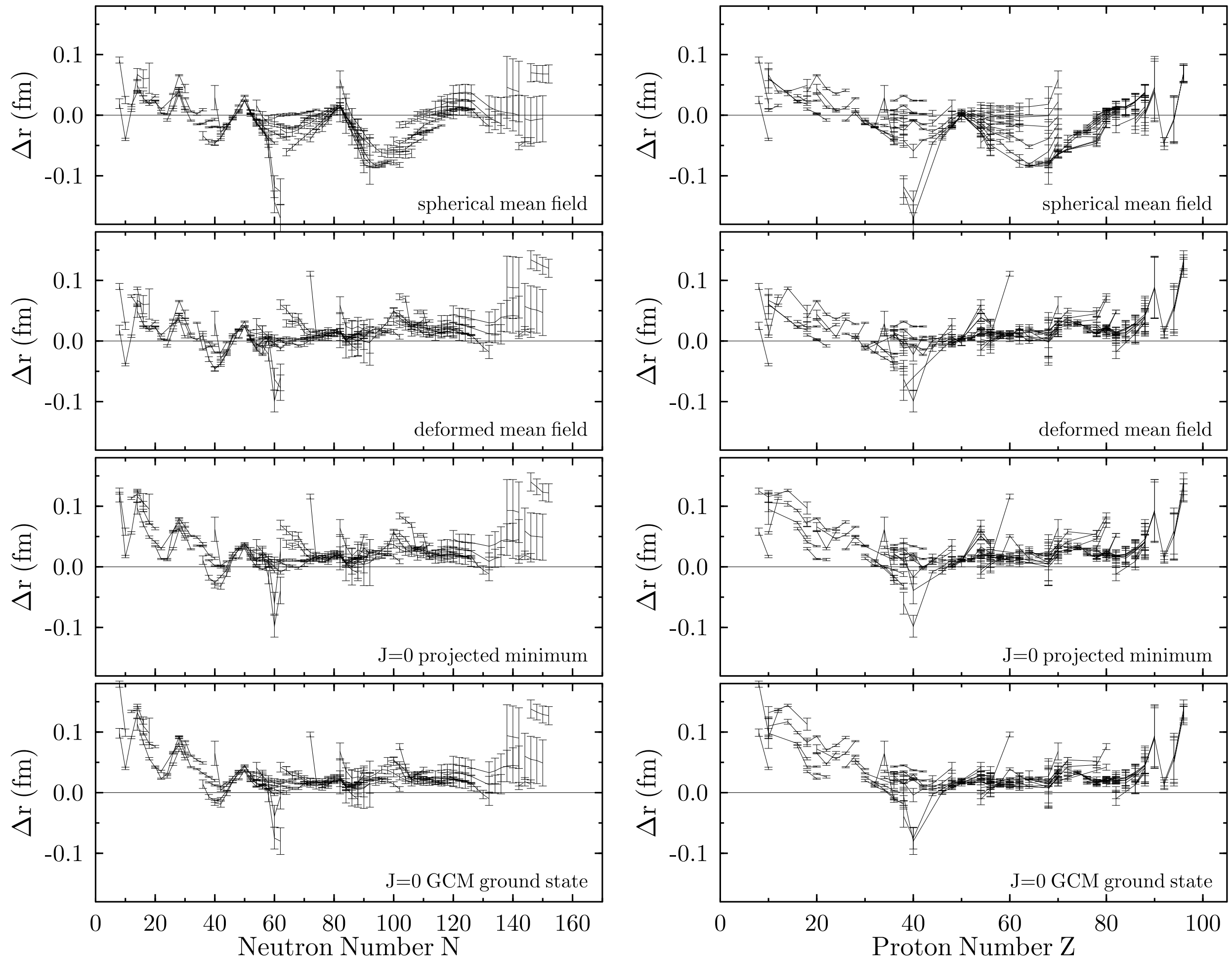
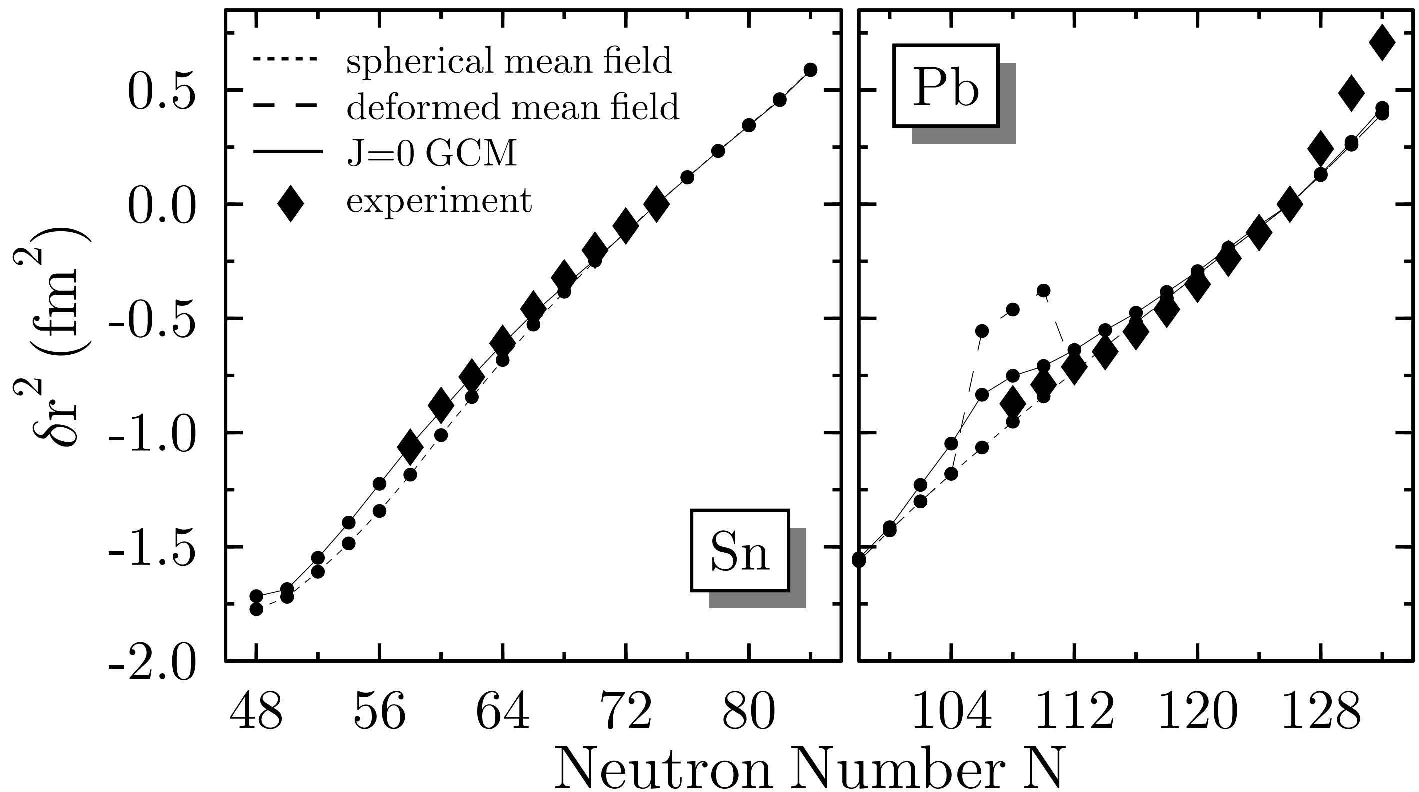
Systematics of rms charge radii



data taken from I. Angeli, Atom. Data Nucl. Data Tables **87**, 185 (2004).

M. B., G. F. Bertsch, P.-H. Heenen, nucl-th/0508052

Isotopic shifts of charge ms radii



$$\delta r_c^2(N,Z) = r^2(N,Z) - r^2(N,Z_0)$$

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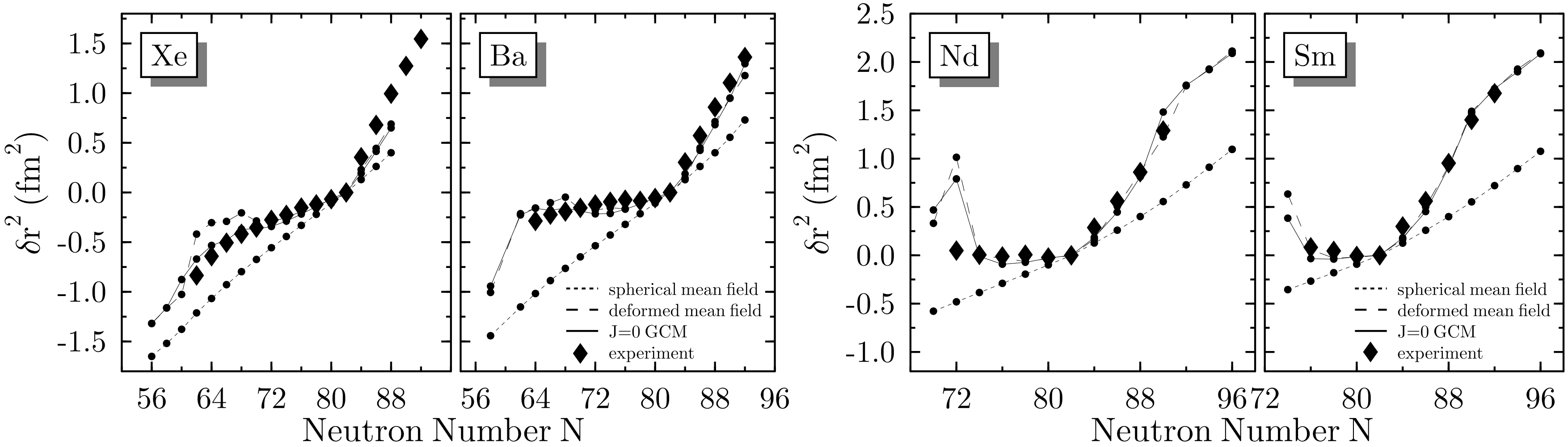
Isotopic shifts of charge ms radii



$$\delta r_c^2(N, Z) = r^2(N, Z) - r^2(N, Z_0)$$

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Status of the Project

- Configuration mixing of symmetry-restored mean-field states provides a tool to analyze and predict ground-state and spectroscopic properties
- The method keeps the intuitive features of mean-field models (shapes, shells) and adds new features as excitation spectra, transition moments, etc, and allows the description of additional phenomena as shape coexistence.
- The method can be applied to *all (but the lightest)* nuclei using a *universal* interaction.
- Adding beyond-mean-field quadrupole correlations improves the systematics of binding energies, in particular around magic numbers.
- For light nuclei, the beyond-mean-field quadrupole correlation energy is of the same order as the mean-field quadrupole deformation energy.

- The density of excited states is too low with the implementation of the model assuming axial symmetry and time-reversal-invariant states.
- Certain excitation modes cannot (yet) be described.
- Going beyond the mean-field does not (yet) cure all deficiencies of mean-field models, as the current effective interactions cannot be expected to be the best starting point to do so.

$\Rightarrow$ Present results are encouraging, but there is a lot of work left to be done.

Outlook: Possible Future Developments

Additional generator coordinates:

non-axial quadrupole moment	⇔	full 5d quadrupole dynamics	*work in progress*
"pairing gaps"	⇔	dynamical pairing	*work in progress*
octupole deformation	⇔	octupole vibrations	*for the moment without J projection but with Π projection*

- choice of generator coordinates and the collective path
- role of diabatic states
- Effective Interaction:
  - — improve fit protocol and strategy
  - — refit with ground-state correlations
  - — revisit density dependence — effective mass — spin-orbit interaction — . . .
  - — establish link to bare nucleon-nucleon interaction
- what about odd-A and odd-odd nuclei?

Acknowledgements

The work presented here would have been absolutely impossible without my collaborators

Paul-Henri Heenen, PNTPM Université Libre de Bruxelles, Belgium
George F. Bertsch, INT Seattle, USA
Paul Bonche, CEA Saclay, France
Thomas Duguet, NSCL/Michigan State University, USA
Hubert Flocard, CSNSM Orsay, France

Over the years, this work was supported in parts by the U.S. Department of Energy under Grant DE–FG02–00ER41132 (INT) and Grant W–31–109–ENG-38 (Argonne National Laboratory), by the National Science Foundation under Grant No. PHY–0456903, the Belgian Science Policy Office under contract PAI P5–07, and an Individual Marie-Curie scholarship of the European Commission.

The numerical calculations were performed in parts at the National Energy Research Scientific Computing Center (NERSC), supported by the U.S. Department of Energy under Contract No. DE–AC03–76SF00098, and computing centers at the Université Libre de Bruxelles (Belgium), as well as Grenoble and Bruyeres-la-chatel (France).

. . . to be continued