Correlation Energies by the Projected Generator Coordinate Method

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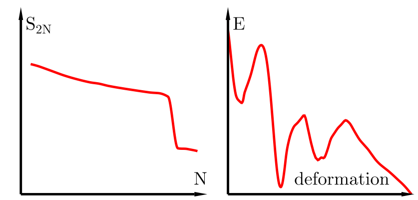
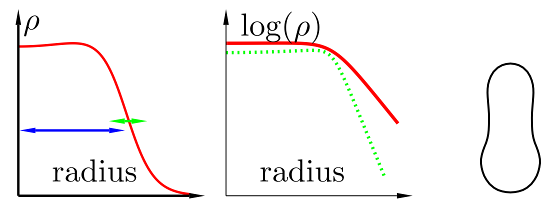
Self-Consistent Mean Field Models I: Typical Applications

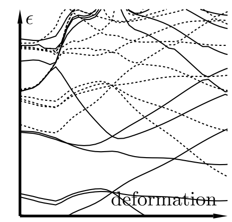
- masses / binding energies
  also separation energies, Q values, etc.
- deformation energy surfaces
  from constrained calculations $\delta(\mathcal{E} - \lambda\langle\hat{Q}\rangle) = 0$



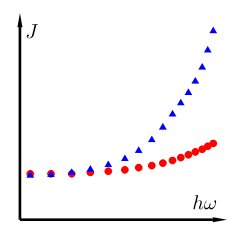
- radial density distribution
  rms radius (charge, neutron), neutron skin
  surface thickness, charge form factor
- spatial density distribution
  multipole moments (well-deformed nuclei only)



- single-particle energies (with some limitations)
  also spin-orbit splittings
  shell structure far from stability, shell quenching
  Superheavy nuclei (large mass and charge number)
  neutron-rich nuclei (large asymmetry, closeness of the continuum)



- rotational bands of well-deformed nuclei at large angular momentum
  from cranking calculations $\delta(\mathcal{E} - \omega_i\langle\hat{J}_i\rangle) = 0$



M. Bender, P.-H. Heenen, P.-G. Reinhard, Rev. Mod. Phys. 75 (2003) 121.

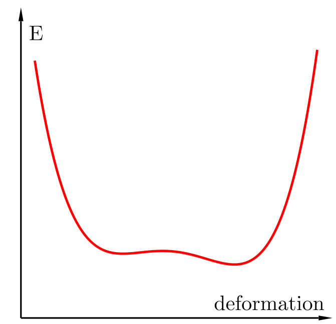
Self-Consistent Mean Field Models II: Prospects and Problems

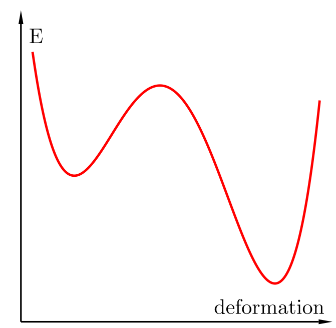
- self-consistency, full model space of occupied states
- universal effective interaction
- Intuitive interpretation in terms of $\begin{cases} \text{shapes of a nuclear liquid} \\ \text{shells of single-particle states} \end{cases}$
- nuclei are described in a body-fixed intrinsic frame
- symmetry breaking. 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

$\Rightarrow$ nice: adds mp-nh and p-p shell-model correlations
$\Rightarrow$ bad: still missing correlations related to symmetry restoration
$\Rightarrow$ difficult connection to the lab frame for spectroscopic observables

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





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

- particle-number projection

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

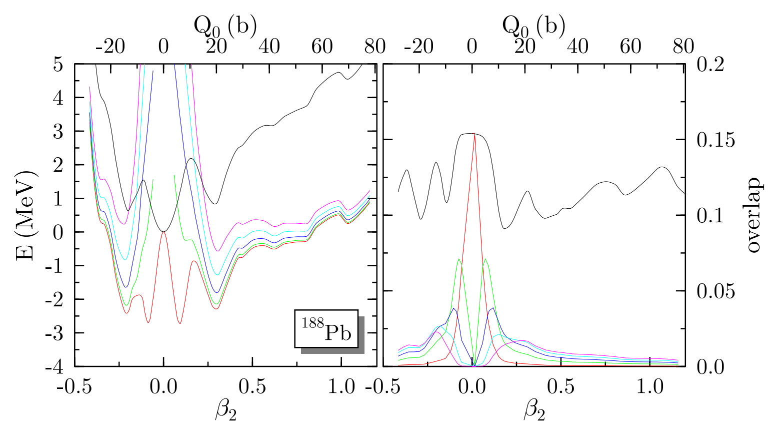
- angular-momentum projection

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

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

Significantly simplified for axial states

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



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

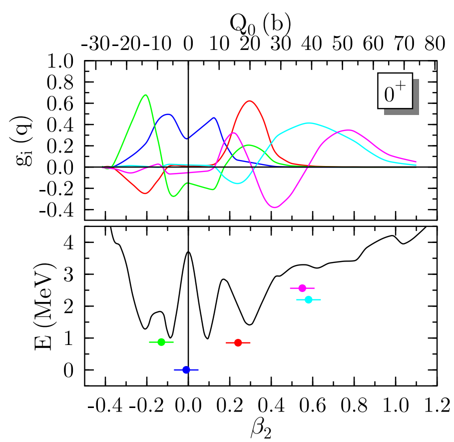
mixed projected many-body state: $|JMk\rangle = \sum_q f_{Jk}(q)\,|JMq\rangle$ $\quad \begin{cases} f_{J,k}(q) & \text{weight function} \\ |JMq\rangle & \text{projected mean-field state} \end{cases}$

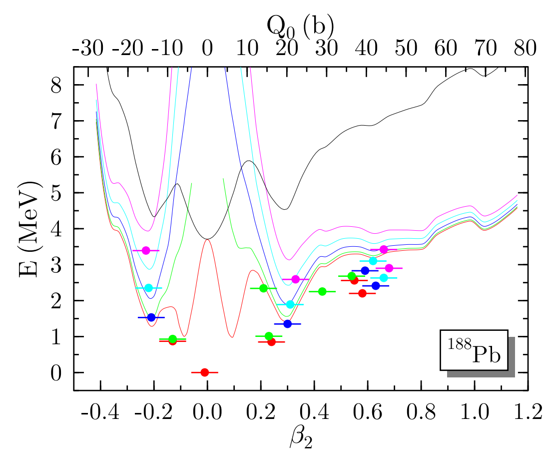
stationarity: $$\frac{\delta}{\delta f^*_{Jk}} \frac{\langle JMk|\hat{H}|JMk\rangle}{\langle JMk|JMk\rangle} = 0$$

$\Rightarrow$ Hill-Wheeler equation

$$\sum_q \left[\mathcal{H}_J(q,q') - E_k\,\mathcal{I}_J(q,q')\right] f_{J,k}(q') = 0 \qquad \begin{cases} \mathcal{H}_J(q,q') = \langle JMq|\hat{H}|JMq'\rangle & \text{Hamiltonian kernel} \\ \mathcal{I}_J(q,q') = \langle JMq|JMq'\rangle & \text{norm kernel} \end{cases}$$

- correlated ground state
- excited states (from orthogonalisation to the ground state)





Current Implementation of the Model

- configuration mixing of particle-number and angular-momentum projected states
- time-reversal invariant self-consistent HF+BCS or HFB states
- approximate particle-number projection before variation à la Lipkin-Nogami
- representation of the single-particle states on a 3d mesh
- restriction to axially and reflection-symmetric shapes $\Rightarrow$ J even, $K = 0$, $P = +1$
- mass quadrupole moment serves a generator coordinate
- Skyrme parameterization SLy4 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. Bender, P.-H. Heenen, Nucl. Phys. A713 (2003) 390
^{32}S, ^{36,38}Ar, ^{40}Ca	M. Bender, H. Flocard, P.-H. Heenen, Phys. Rev. C 68 (2003) 044321
^{186}Pb	T. Duguet, M. Bender, P. Bonche, P.-H. Heenen, Phys. Lett. B559 (2003) 201
$^{182-194}$Pb	M. Bender, P. Bonche, T. Duguet, P.-H. Heenen, Phys. Rev. C 69 (2004) 064303
^{240}Pu	M. Bender, P.-H. Heenen, P. Bonche, submitted to Phys. Rev. C.

Going Beyond the Mean Field Made Simple

- Full calculation requires

$$\left.\begin{array}{l} n_J \approx 5\dots15 \text{ rotated states} \\ n_q \approx 7\dots25 \text{ deformations} \end{array}\right\} \Rightarrow \quad n_J \times \frac{n_q(n_q+1)}{2} \approx 150\dots5000 \text{ mixed configurations}$$

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

$\Rightarrow$ 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

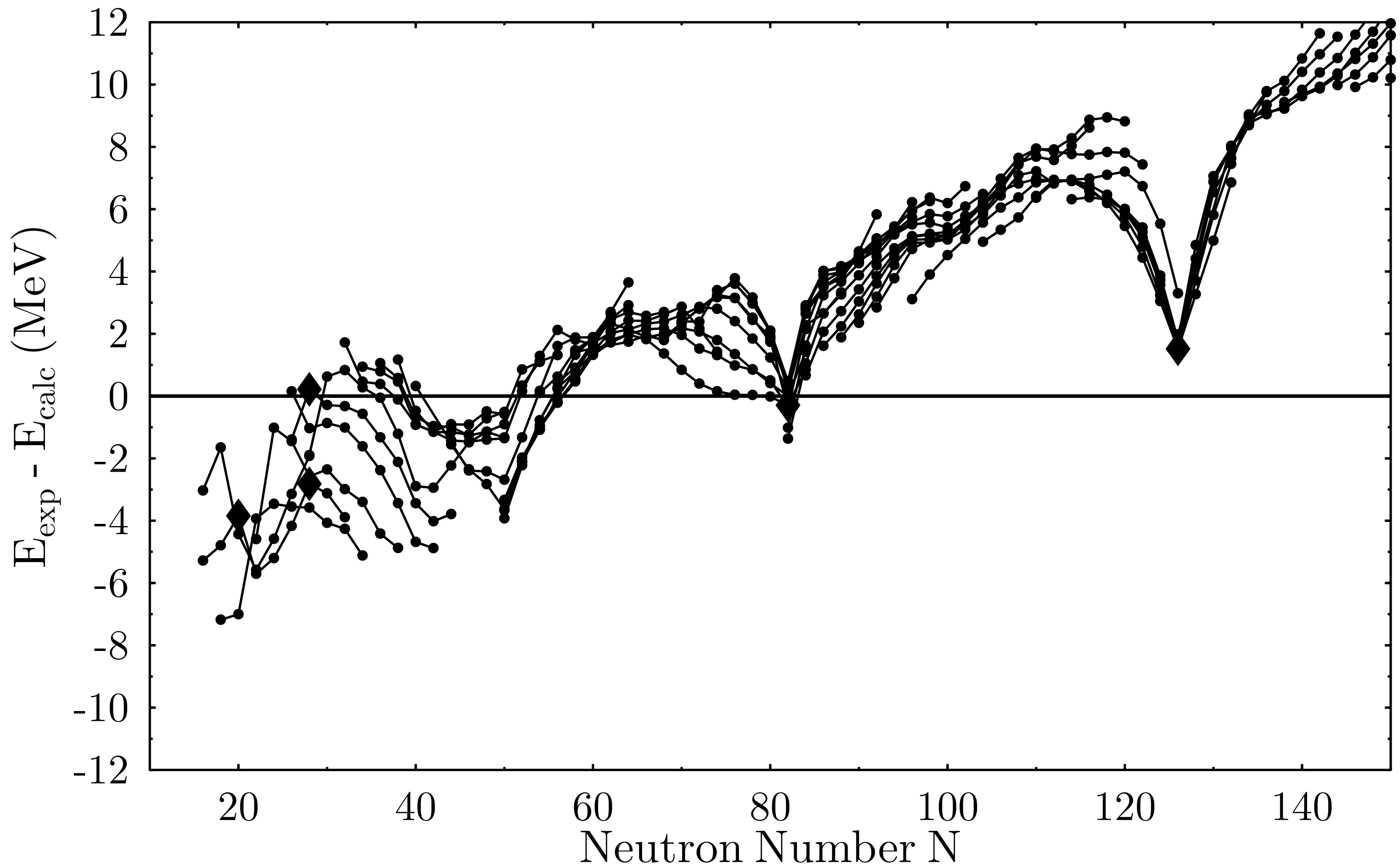
$\Rightarrow$ $n_J \times [n_q + (n_q - 1)] \approx 26\dots100$ calculated matrix elements

$\Rightarrow$ Accuracy better than 300 keV $\Rightarrow$ sufficient for study of systematics of quadrupole correlation energies

$\Rightarrow$ emphasis on ground state — most information on spectroscopy is lost

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

Masses from Mean-Field Calculations



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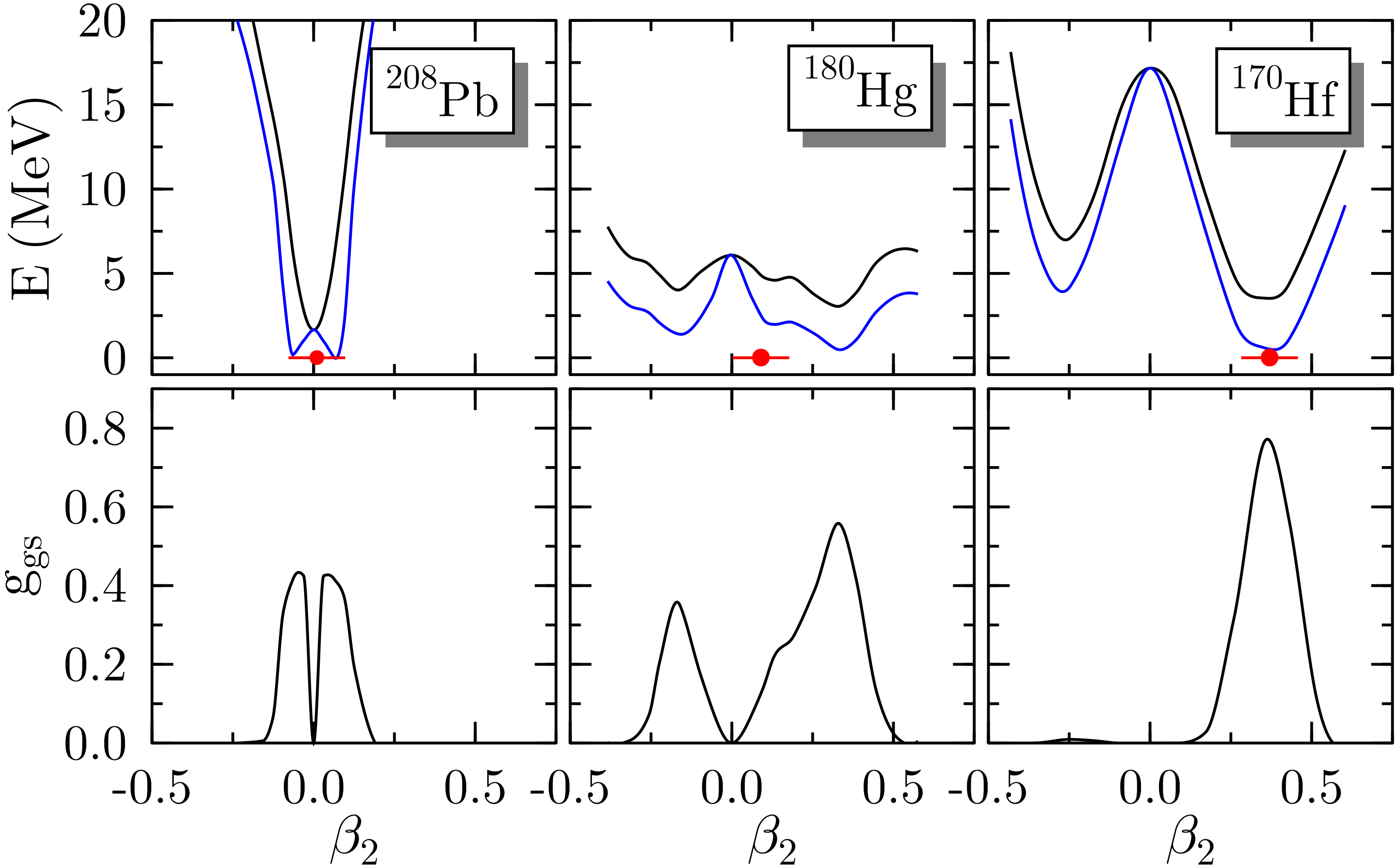
Typical Situations



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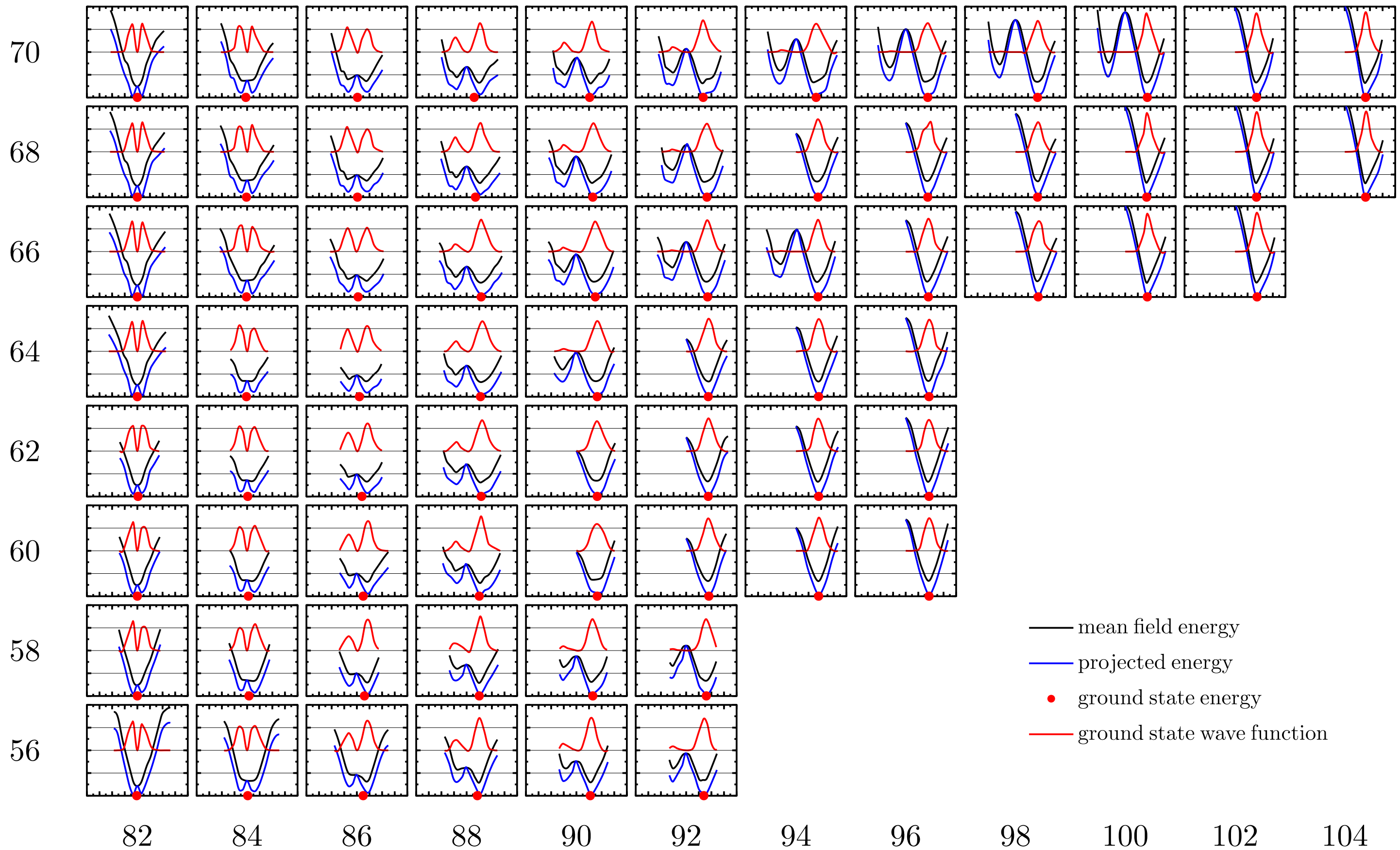

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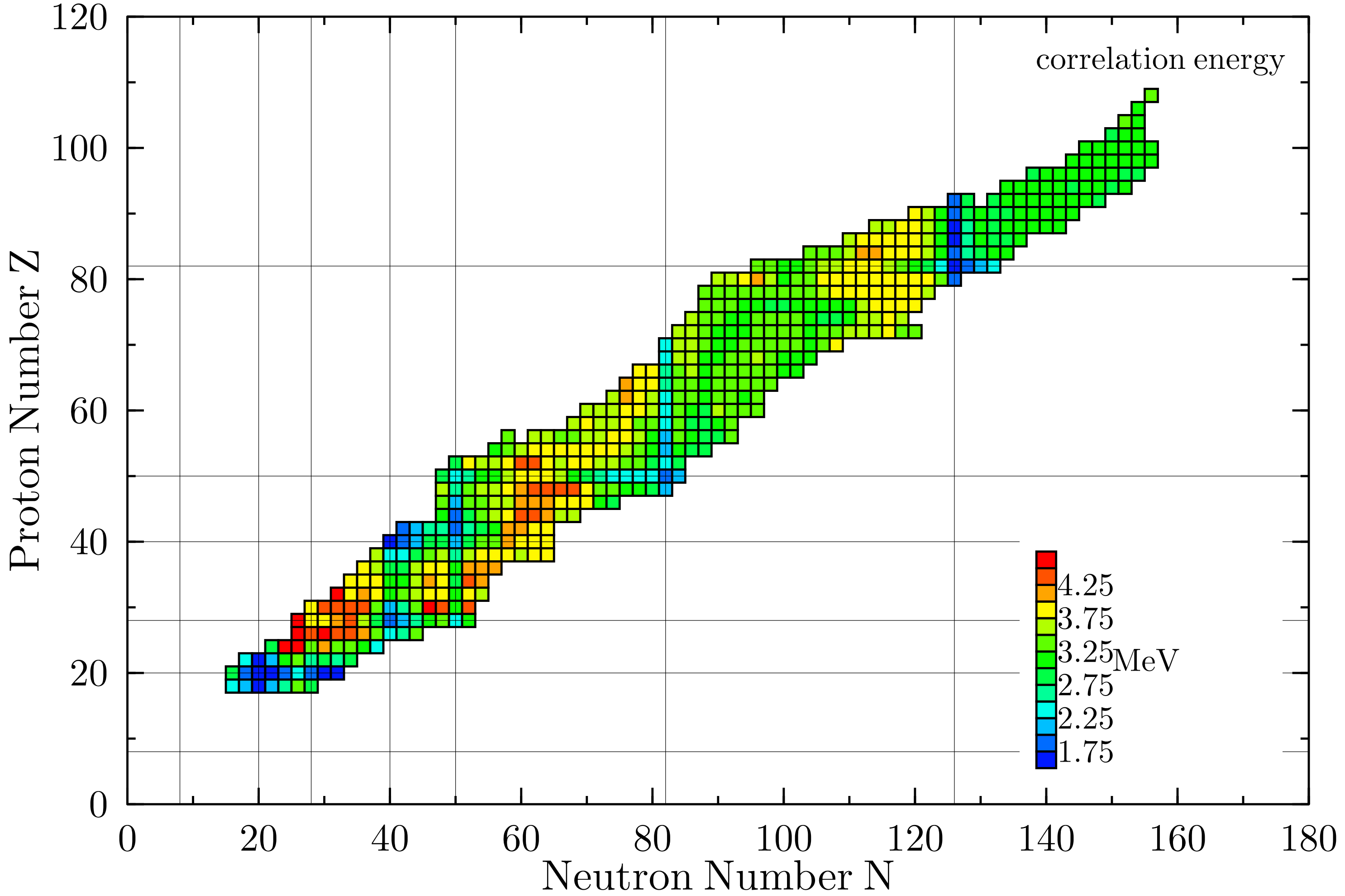
Quadrupole Correlation Energy from Projection and Configuration Mixing



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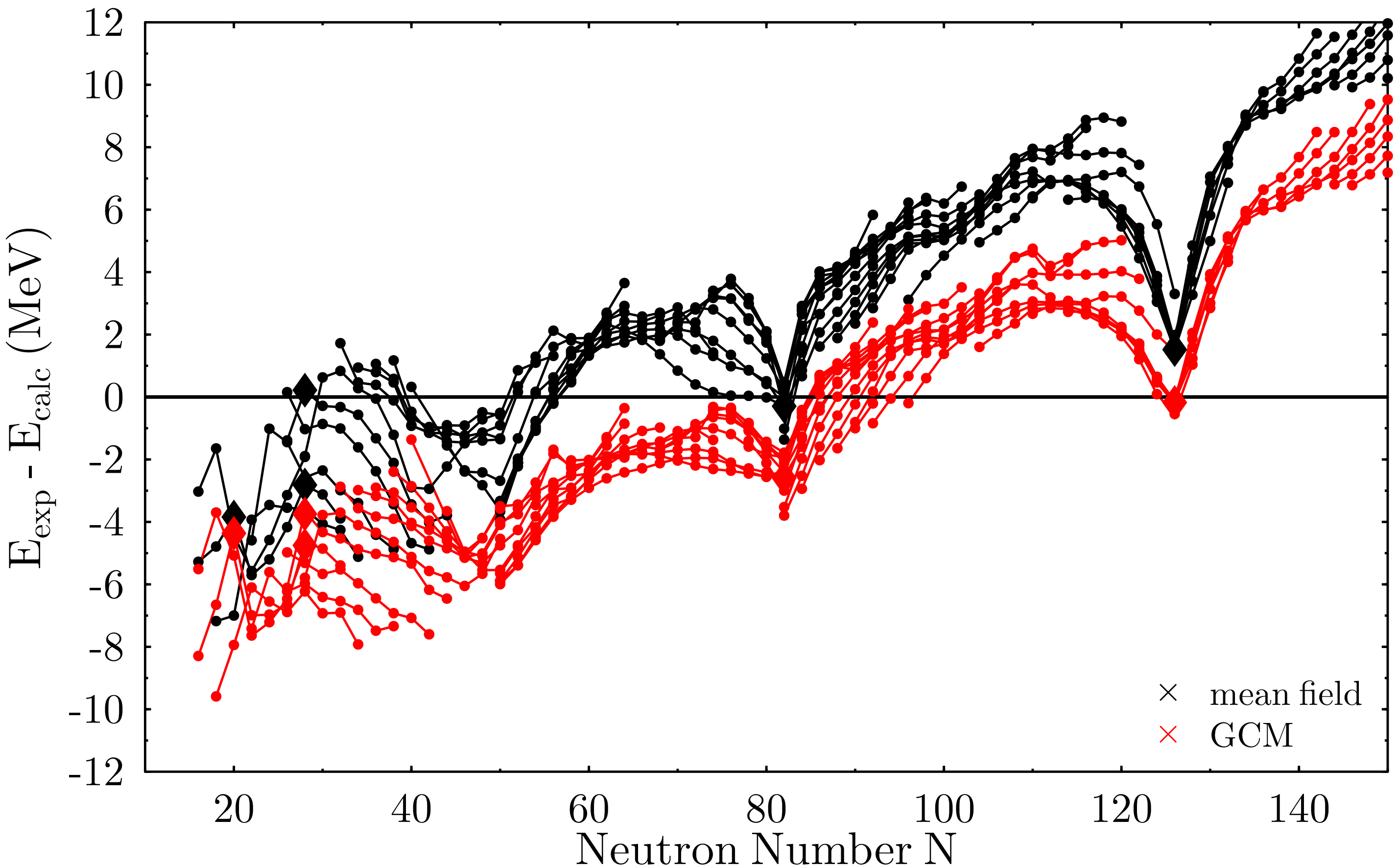
Masses including Correlations



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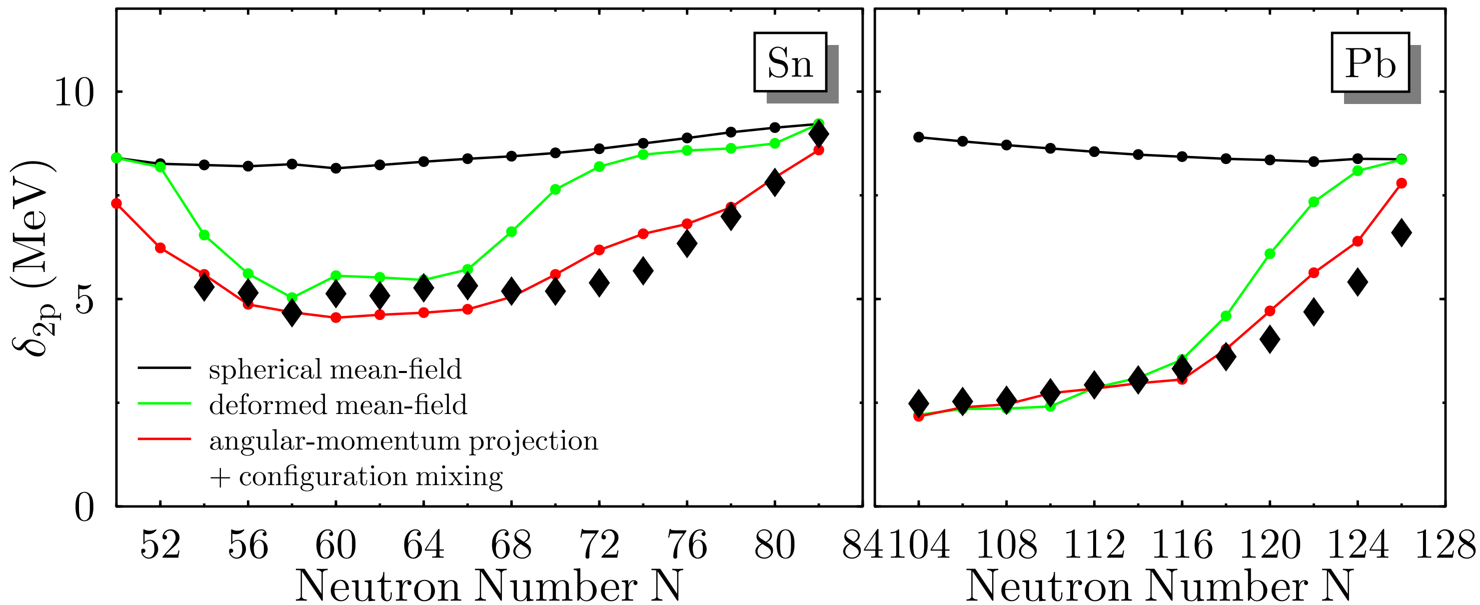
Systematics of Mass-Difference Formulas



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

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

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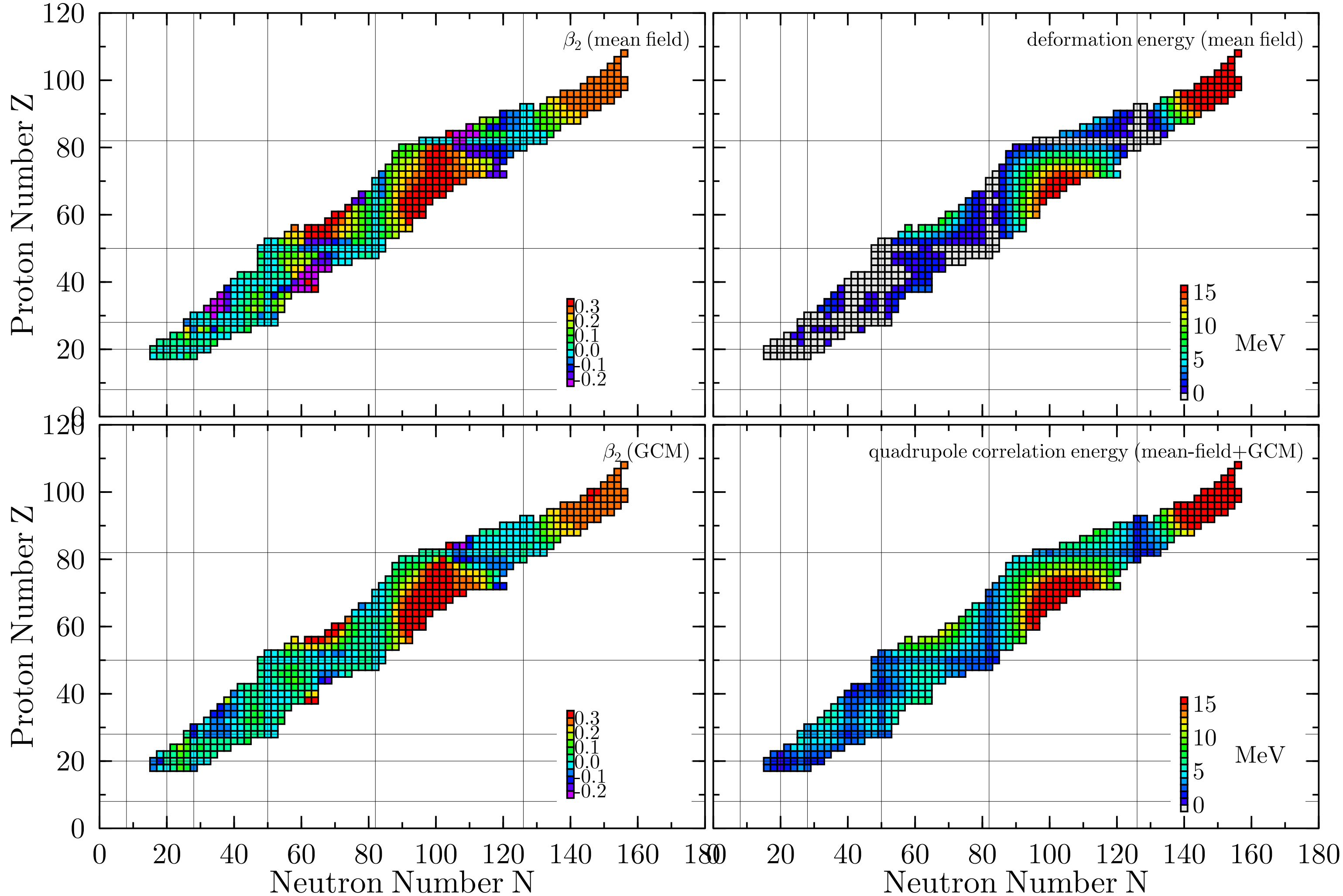
Intrinsic Deformation and Quadrupole Correlation Energy



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Summary

- Configuration mixing of symmetry-restored mean-field states provides a tool to analyze and predict ground-state properties and excited states
- 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 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.

Outlook: Current and Future Developments

- Modeling

	(quadrupole) deformation	pairing
shell-model correlation	mp-nh	p-p
broken symmetry	rotational	particle number
exact projection after variation	angular momentum	particle number
approximate restoration before variation	cranking	Lipkin-Nogami
dynamical correlation	quadrupole vibrations	pairing vibrations

- Configuration space
  - — octupole deformation ⇔ parity
  - — choice of generator coordinates (constraints, triaxiality)
  - — role of diabatic states
- Effective Interaction
  - — isovector properties — density dependence — spin-orbit interaction — . . .
  - — spin-spin and spin-isospin interaction
  - — connection to ab-initio calculations

. . . support your local theorist and stay tuned.