The importance of nuclear deformation in low-energy nuclear phenomenology and models

Benjamin Bally

ESNT workshop - Saclay - 20/09/2022

Outline of the presentation

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Symmetries of the nuclear Hamiltonian H

Definition

Let $G \equiv \{g\}$ be a group with a unitary representation $R(g)$

If $\forall\, g \in G,\ R(g) H R^{-1}(g) = H \quad \Rightarrow\ G$ is a symmetry group of H

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Physical symmetry	Group	Quant. numb.
Particle-number inv.	$U(1)_Z \times U(1)_N$	N, Z
Rotational inv.	$SU(2)_A$	J, M_J
Parity inv.	Z_{2A}	π
Translational inv.	T^3_A	$\vec{P}$
Exchange of particles	$S_Z \times S_N$	-1, -1
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- Nuclear eigenstates have good quantum numbers: $|\Psi_{\epsilon}^{JM_J\pi}\rangle$

Properties of the eigenstates

- Transformation under rotation (Euler angles ≡ α, β, γ)

$$R(\alpha, \beta, \gamma)|\Psi_{\epsilon}^{JM\pi}\rangle = \sum_{K=-J}^{J} D^{J}_{KM}(\alpha, \beta, \gamma)|\Psi_{\epsilon}^{JK\pi}\rangle$$

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- Expectation value for $Q_{\lambda\mu} \equiv r^{\lambda} Y_{\lambda\mu}(\theta,\phi)$ with $\lambda \in \mathbb{N}$ and $\mu \in [\![-\lambda,\lambda]\!]$

$$\langle\Psi_{\epsilon}^{JM\pi}|Q_{\lambda\mu}|\Psi_{\epsilon}^{JM\pi}\rangle \neq 0 \Leftrightarrow \begin{cases} J \in [\![|J-\lambda|, J+\lambda]\!] \\ \mu = 0 \\ (-1)^{\lambda} = 1 \end{cases}$$

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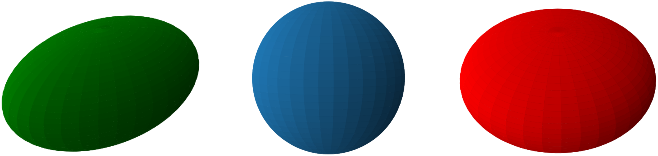
- Example of $J = 0$ states
  - ◇ $\forall(\alpha,\beta,\gamma)$, $R(\alpha,\beta,\gamma)|\Psi_\epsilon^{J=0M=0\pi}\rangle = |\Psi_\epsilon^{J=0M=0\pi}\rangle$
  - ◇ If $\lambda, \mu \neq 0$, $\langle\Psi_\epsilon^{J=0M=0\pi}|Q_{\lambda\mu}|\Psi_\epsilon^{J=0M=0\pi}\rangle = 0$
  - ◇ Ground states of all even-even nuclei have $J = 0$

Intrinsic deformations

- Nuclear models often rely on the picture of intrinsic shapes



Intrinsic deformations: parametrization

- Parametrization of the nuclear radius (surface)

$$R(\theta,\phi) = R_0 \left\{ 1 + \sum_{\lambda} \sum_{\mu=-\lambda}^{\lambda} a_{\lambda\mu} Y_{\lambda\mu}(\theta,\phi) \right\}$$

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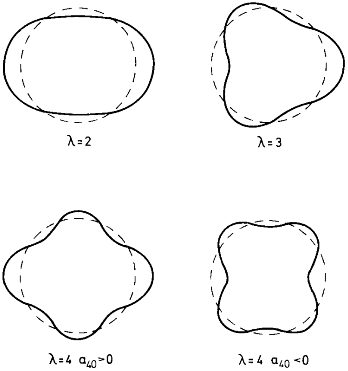
- Small values of λ are the most important!



Ring and Schuck, The Nuclear Many-Body Problem (1980)

Intrinsic deformations: quadrupole

- Quadrupole ($\lambda = 2$) is the most important!

$$R(\theta,\phi) = R_0 \left\{1 + \beta_S \cos(\gamma_S) Y_{20}(\theta,\phi) + \sqrt{2}\beta_S \sin(\gamma_S) \Re\left[Y_{22}(\theta,\phi)\right]\right\}$$

- Usual parametrization with β_S and γ_S

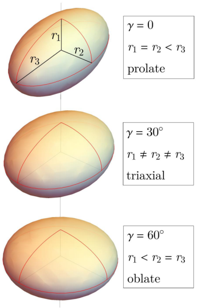
$$a_{\lambda -\mu} = (-1)^{\lambda} a_{\lambda\mu}$$

$$a_{2-1} = a_{21} = 0$$

$$\beta_S = \frac{4\pi}{3R_0^2 A}\sqrt{a_{20}^2 + 2a_{22}^2}$$

$$\gamma_S = \arctan\left(\frac{\sqrt{2}a_{22}}{a_{20}}\right)$$

deformed nucleus ($\beta > 0$)



Phenomenology

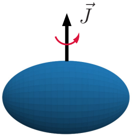
- Explanation of many phenonmenon makes use of intrinsic deformations
  - Excitation spectra (e.g. rotational bands)
  - Values of electromagnetic moments and transitions
  - Trends of observables with $A/N/Z$ (e.g. binding energes or charge radii)
  - Presence of competing states with same J^π but different structure (shape coexistence)
  - Dynamic of nuclear fission
  - ...

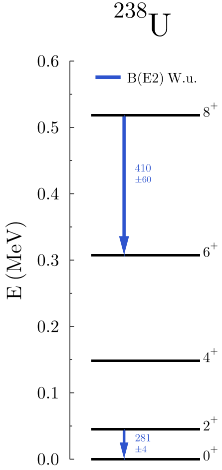
Rotational bands

- Sequence of levels can be grouped into rotational bands

$$E(J) = \frac{J(J+1)}{2\mathcal{I}}$$

- Semi-classical picture: deformed nucleus rotating





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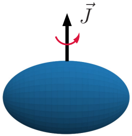
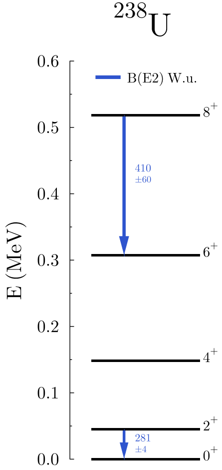


- Rigid rotor limit: $R_{42} = \frac{E(4)}{E(2)} = 3.33$
  For ^{238}U: $R_{42} = 3.30$



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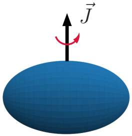

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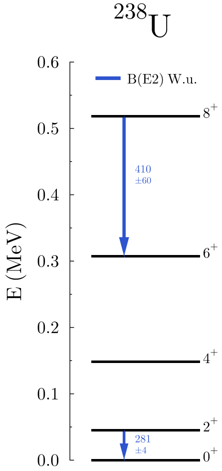
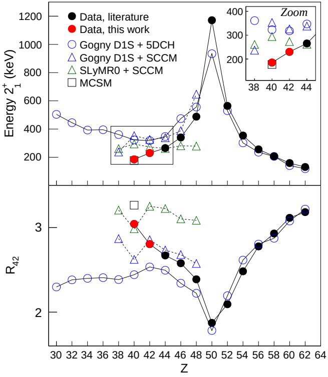
- Very collective electromagnetic transitions



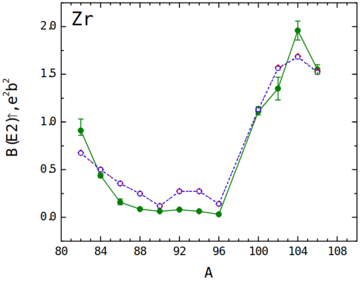
Evolution of $E(2_1^+)$ and $B(E2)$

- Trends to identify the evolution with $A/Z/N$

- For example: $E(2_1^+)$ and $B(E2:2_1^+ \to 0_1^+) = \frac{1}{5}B(E2:0_1^+ \to 2_1^+)$



Paul *et al.*, Phys. Rev. Lett. 118, 032501 (2017)



Pritychenko *et al.*, Nucl. Phys. A 962, 73 (2017)

Electric quadrupole moment

- Electric quadrupole moment

$$Q_s = \langle \Psi_\epsilon^{J\pi} | E_{20} | \Psi_\epsilon^{J\pi} \rangle \equiv \langle \Psi_\epsilon^{J\pi} | q r^2 Y_{20}(\theta, \phi) | \Psi_\epsilon^{J\pi} \rangle$$

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- $Q_s = 0$ for $J = 0$ and 1/2 states
  → all the ground states of even-even nuclei have $J = 0$

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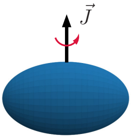
Axial rigid-rotor: assignement of β

- Semi-classical picture: deformed nucleus rotating



- Intrinsic deformation β_r assigned from intra-band $E2$ transitions

$$\beta_r(0_1^+) = \frac{4\pi\sqrt{5}}{3ZR_0^2}\sqrt{B(E2 : 2_1^+ \to 0_1^+)} = \frac{4\pi}{3ZR_0^2}\,|\langle 0_1^+||E_2||2_1^+\rangle|$$

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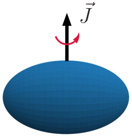

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- For ^{238}U: $\beta_r(0_1^+) = 0.289$

Asymmetric rigid-rotor: assignement of γ

- Davydov's model
  Davydov and Filippov, Nucl. Phys. A 8, 237 (1958)

- Intrinsic deformation γ_d assigned from ratio of energies

$$\frac{E(2_2^+)}{E(2_1^+)} = \frac{1 + \sqrt{1 - \frac{8}{9}\sin^2(3\gamma_d)}}{1 - \sqrt{1 - \frac{8}{9}\sin^2(3\gamma_d)}}$$

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- For ^{238}U: $\gamma_d(0_1^+) = 8.6°$

  $E(2_1^+) + E(2_2^+) = 1011$ keV $\approx E(3_1^+) = 1059$ (or 1106) keV

Kumar quadrupole parameters

- Determine parameters of equivalent ellipsoid from E2 matrix elements (tensor operator E_2 with components $E_{2\mu} = qr^2 Y_{2\mu}$)

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$$\beta_k(0_1^+) \approx \left(\frac{4\pi}{3R_0^2 A}\right) \left[\sqrt{5} \langle \Psi_1^{0^+} | \left[E_2 \times E_2\right]_0 | \Psi_1^{0^+} \rangle \right]^{1/2}$$

$$\cos\left[3\gamma_k(0_1^+)\right] \approx -\sqrt{\frac{35}{2}} \frac{\langle \Psi_1^{0^+} | \left[\left[E_2 \times E_2\right]_2 \times E_2\right]_0 | \Psi_1^{0^+} \rangle}{\left[\sqrt{5} \langle \Psi_1^{0^+} | \left[E_2 \times E_2\right]_0 | \Psi_1^{0^+} \rangle \right]^{3/2}}$$

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- The right hand side matrix elements can be written

$$\langle \Psi_1^{0^+} | \left[E_2 \times E_2 \right]_0 | \Psi_1^{0^+} \rangle = \frac{1}{\sqrt{5}} \sum_{\epsilon_1} \langle \Psi_1^{0^+} || E_2 || \Psi_{\epsilon_1}^{2^+} \rangle \langle \Psi_{\epsilon_1}^{2^+} || E_2 || \Psi_1^{0^+} \rangle$$

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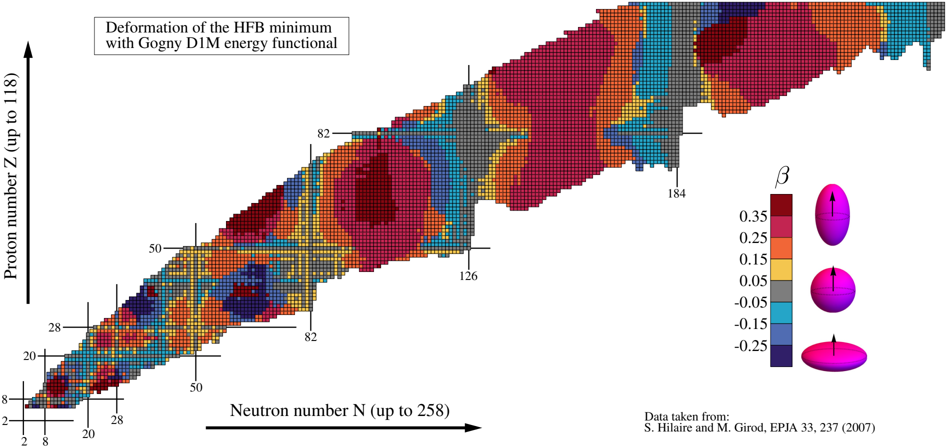
- Capture strong collective correlations keeping the simple one-body picture

Deformation is (almost) ubiquitous



Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)

Constrained calculations

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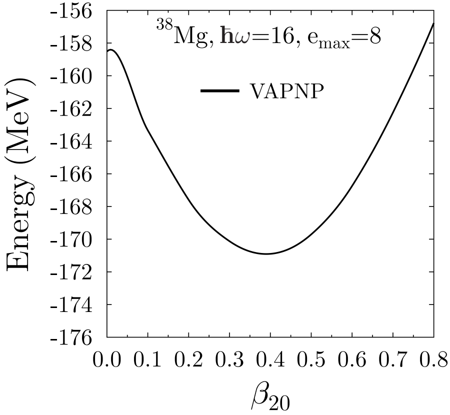

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- Same for other values of λ, μ

Energy Density Functional (EDF)

- The energy is represented as a functional of one-body densities

$$\langle\Phi|H|\Phi\rangle \equiv E[\rho,\kappa,\kappa^*] \text{ with } \begin{cases} \rho_{ij} = \langle\Phi|a_j^\dagger a_i|\Phi\rangle \\ \kappa_{ij} = \langle\Phi|a_j a_i|\Phi\rangle \\ \kappa_{ij}^* = \langle\Phi|a_i^\dagger a_j^\dagger|\Phi\rangle \end{cases}$$

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- But EDF philosophy goes further
  - Form of $E[\rho, \kappa, \kappa^*]$ is general (e.g. ρ^α with $\alpha \notin \mathbb{N}$)
  - Parameters of $E[\rho, \kappa, \kappa^*]$ fitted to experimental data

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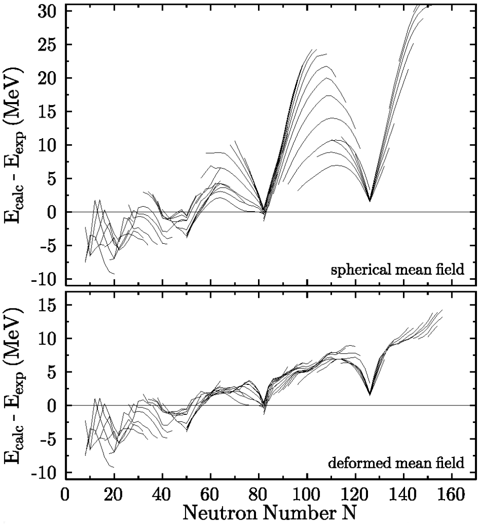
  - ◇ Mathematical problems when going beyond the mean field (BMF)
  - ◇ Research field is stagnant

Influence of deformation: binding energies



Bender *et al.*, Phys. Rev. C 73, 034322 (2006)

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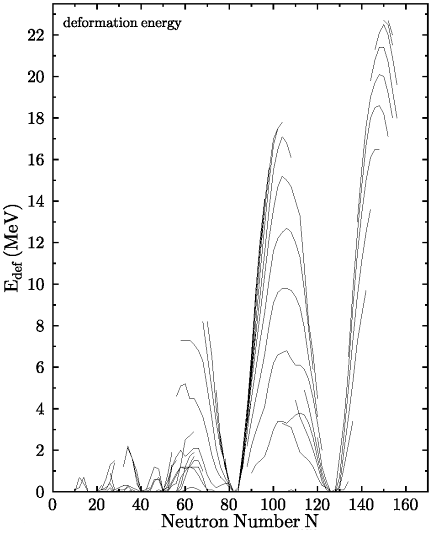

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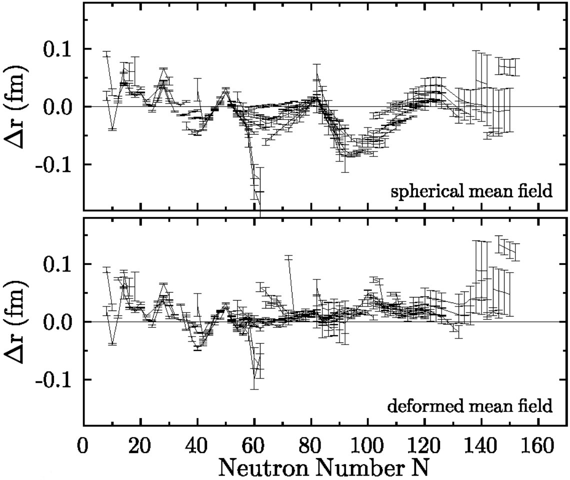
Influence of deformation: radii



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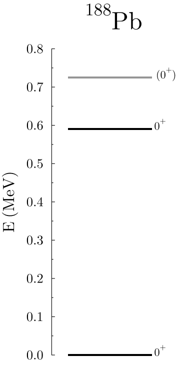

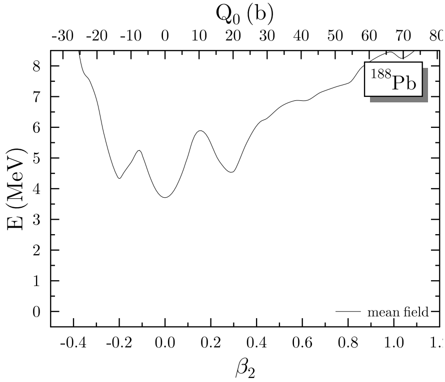

Bender *et al.*, Phys. Rev. C 69, 064303 (2004)

Symmetry-breaking and quantum numbers

- Deformed solutions break the symmetries of H

$$|\Phi(q_i)\rangle = \sum_{JM\pi} \sum_{\epsilon} c_{\epsilon}^{JM\pi}(q_i) |\Theta_{\epsilon}^{JM\pi}(q_i)\rangle \quad \Rightarrow \text{ unphysical in nuclei}$$

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  - ◇ Symmetry-breaking MF $\xrightarrow{\text{reference states}}$ Symmetry-restored BMF

Outline of the presentation

Symmetry projection: method

- Projection operators

$$P^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{4\pi} d\gamma \, D^{J}_{MK}{}^{*}(\alpha,\beta,\gamma)\, R(\alpha,\beta,\gamma)$$

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- Extraction of the components

$$\underbrace{P^J_{MK} P^\pi}_{\text{projection operators}} |\Phi(q_i)\rangle \xrightarrow{\text{projects}} \left\{ \sum_\varepsilon c^{JK\pi}(q_i) |\Theta^{JM\pi}_\varepsilon(q_i)\rangle, K \right\} \xrightarrow{\text{diag. } H} \{ |\Theta^{JM\pi}_\varepsilon(q_i)\rangle, \varepsilon \}$$

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- Projected states

$$|\Theta^{JM\pi}_\varepsilon(q_i)\rangle = \sum_K f^{JM\pi}_{\varepsilon K}(q_i) P^J_{MK} P^\pi |\Phi(q_i)\rangle$$

Symmetry projection: illustration

- Projection operator (angular momentum)

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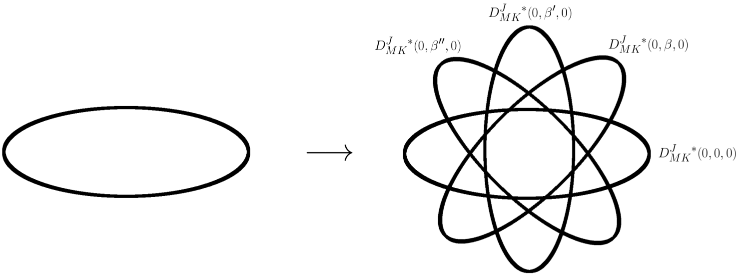
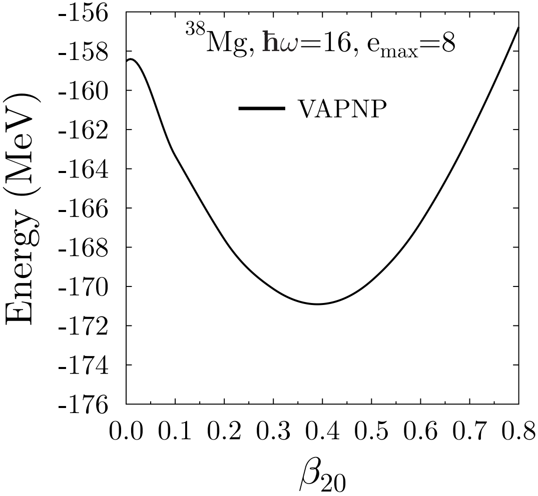


Symmetry projection: example with ^{38}Mg



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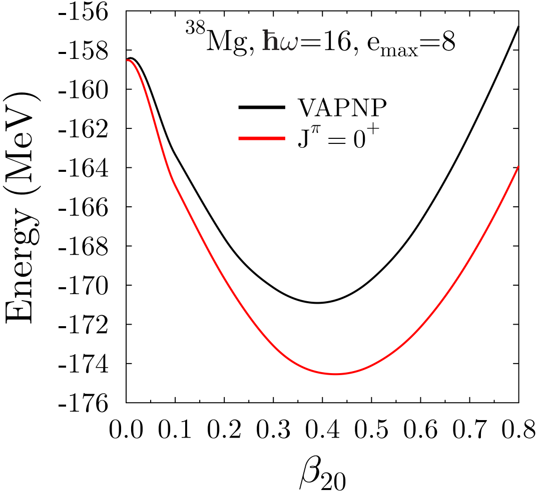

Generator Coordinate Method (GCM): definition

- Trial wave function depends on continuous variables q

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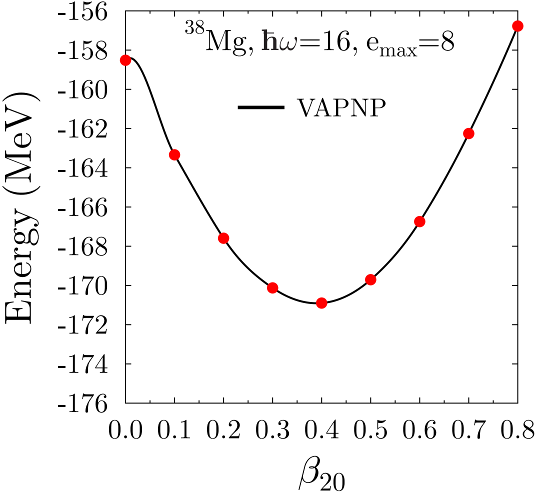
- It translates into solving the generalized eigenvalue problem (GEP)

$$Hf = ENf \quad \text{with} \quad \begin{aligned} H_{ij} &= \langle\Phi(q_i)|H|\Phi(q_j)\rangle \\ N_{ij} &= \langle\Phi(q_i)|\Phi(q_j)\rangle \end{aligned}$$

GCM: illustration



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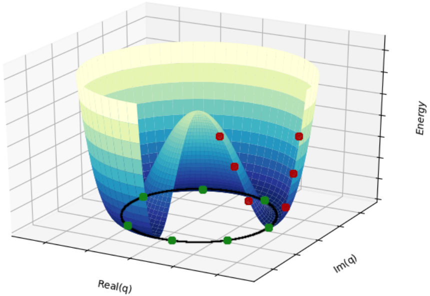
Projected GCM: unified picture

- Order parameter: $q = |q| e^{i \arg(q)}$



Projected GCM: unified picture

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- Example: quadrupole deformations

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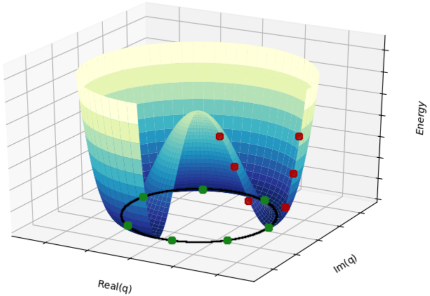
  $\arg(q) \equiv$ Euler angles (α, β, γ)



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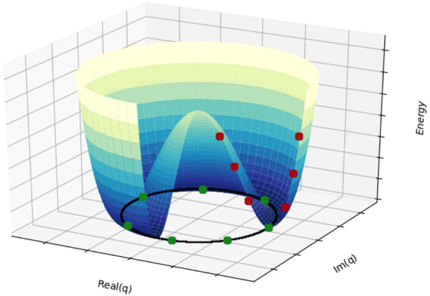
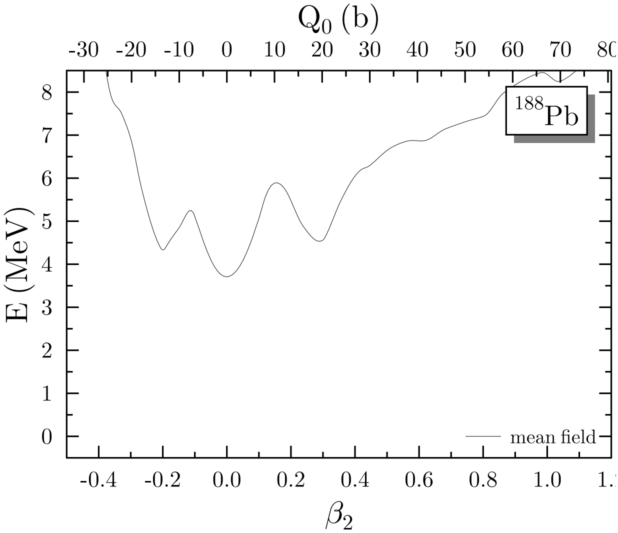


- General ansatz

$$|\Theta_{\epsilon}^{JM\pi}\rangle \equiv \sum_{|q_i|, K} \tilde{f}_{\epsilon}^{JM\pi}(|q_i|, K)\, P^J_{MK} P^{\pi} |\Phi(|q_i|)\rangle$$

Example: ^{188}Pb with SLy6 EDF



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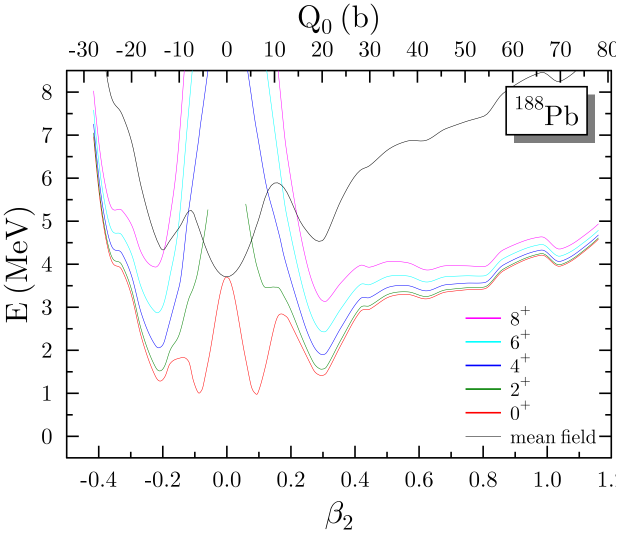

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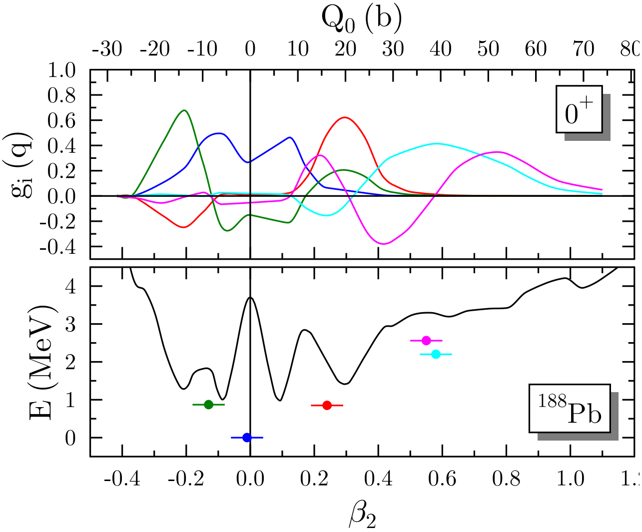

$$\bar{\beta}_i = \sum_{\beta} \beta g_i^2(\beta)$$

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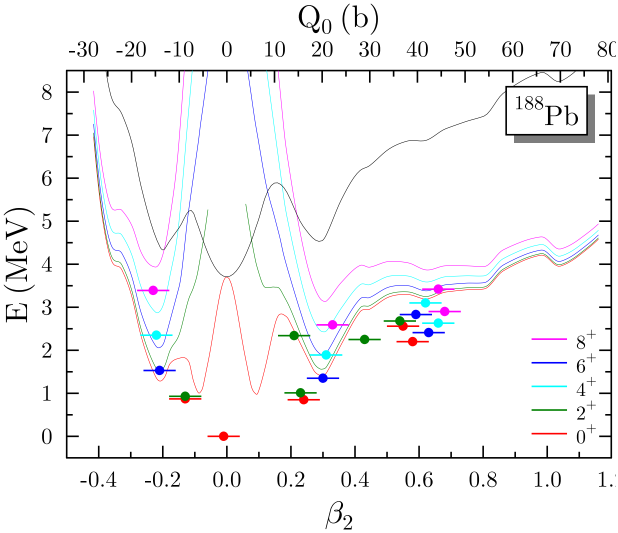

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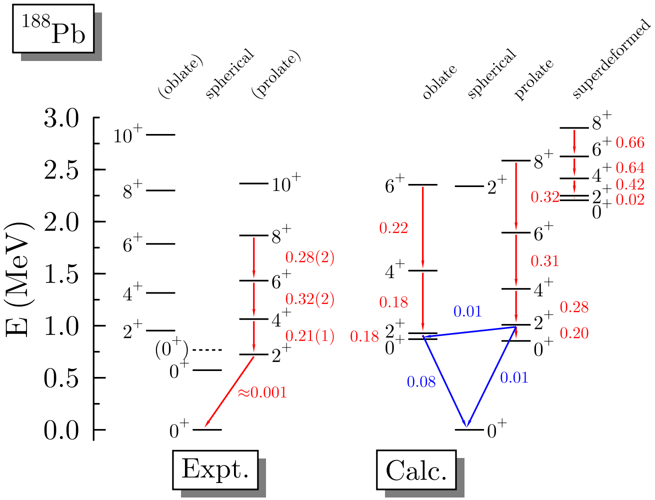

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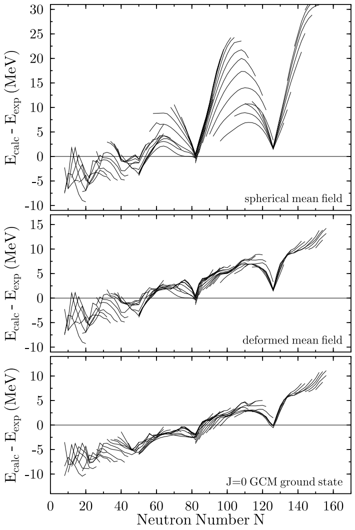
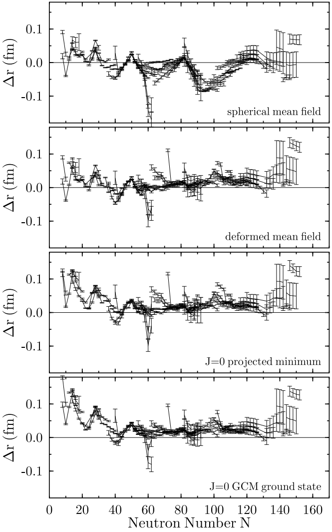
PGCM systematics (SLy4): binding energies



Method	RMS (MeV)
spherical	11.7
deformed	5.3
def. + $J = 0$	4.4
PGCM $J = 0$	4.4

Bender *et al.*, Phys. Rev. C 73, 034322 (2006)

PGCM systematics (SLy4): charge radii



Method	RMS (fm)
spherical	0.037
deformed	0.032
def. + $J = 0$	0.041
PGCM $J = 0$	0.044

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Outline of the presentation

Conclusions

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- Deformed references states have to be projected onto good quantum numbers
- PGCM is an efficient method to include these collective correlations while respecting the symmetries of H
- Recent developments of PGCM in the *ab initio* context

  Yao *et al.*, Phys. Rev. Lett. 124, 232501 (2020)

  Frosini *et al.*, Eur. Phys. J. A 58, 62 (2022)

  Frosini *et al.*, Eur. Phys. J. A 58, 63 (2022)

  Frosini *et al.*, Eur. Phys. J. A 58, 64 (2022)