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Nuclear structure studies based on energy density functionals

Tamara Nikšić
University of Zagreb
the nuclear many-body problem is effectively mapped onto a one-body problem without explicitly involving internucleon interactions.

The exact density functional is approximated with powers and gradients of ground state densities and currents.

Universal density functionals can be extended from relatively light systems to superheavy nuclei and from the valley of stability to the particle drip line.

The coupling parameters of the EDF are fine-tuned to empirical data.

covariant EDFs – built from densities and currents bilinear in the Dirac spinor field of the nucleon.
Basic implementation: self-consistent mean-field method

- produces energy surfaces as functions of intrinsic deformation parameters

The constrained self-consistent mean field method produces semi-classical energy surfaces as functions of intrinsic deformation parameters.

- include static correlations: deformations & pairing
- do not include dynamic (collective) correlations that arise from symmetry restoration and quantum fluctuations around mean-field minima

- includes static correlations: deformations and pairing
- does not include collective correlations originating from symmetry restoration and quantum fluctuations around mean-field minima
Beyond mean-field correlations: Collective Hamiltonian

nuclear excitations determined by quadrupole vibrational and rotational degrees of freedom

\[
H_{\text{coll}} = T_{\text{vib}}(\beta, \gamma) + T_{\text{rot}}(\beta, \gamma, \Omega) + V_{\text{coll}}(\beta, \gamma)
\]

\[
T_{\text{vib}} = \frac{1}{2} B_{\beta\beta} \dot{\beta}^2 + \beta B_{\beta\gamma} \dot{\beta} \dot{\gamma} + \frac{1}{2} \beta^2 B_{\gamma\gamma} \dot{\gamma}^2
\]

\[
T_{\text{rot}} = \frac{1}{2} \sum_{k=1}^{3} I_k \omega_k^2
\]

The entire dynamics of the collective Hamiltonian is governed by the seven functions of the intrinsic deformations \(\beta\) and \(\gamma\): the collective potential, the three mass parameters: \(B_{\beta\beta}, B_{\beta\gamma}, B_{\gamma\gamma}\), and the three moments of inertia \(I_k\).

... collective eigenfunction:

\[
\Psi^{IM}_\alpha(\beta, \gamma, \Omega) = \sum_{K \in \Delta I} \psi^I_{\alpha K}(\beta, \gamma) \Phi^I_{MK}(\Omega)
\]
an intuitive interpretation of mean-field results in terms of intrinsic shapes and single-particle states

the full model space of occupied states can be used; no distinction between core and valence nucleons, no need for effective charges!

Global analysis of quadrupole shape invariants

- Systematic analysis of characteristic signatures of coexisting shapes in different mass regions
- Calculation includes 621 even-even nuclei with $Z,N>10$ and for which $2_{1}^{+}$ state has been determined in experiment

Following criteria for shape coexistence have been used:

- The difference between $\beta_{\text{eff}} \cos(3\gamma_{\text{eff}})$ for the two lowest $0^{+}$ states is large
- The excitation energy of $0_{2}^{+}$ is low in comparison to the excitation energy of the $2_{1}^{+}$ state

Deformation parameters
- Calculated by using the quadrupole shape invariants
Global analysis of quadrupole shape invariants


The lowest-order quadrupole invariants:

\[
q_2(0^+_i) = \sum_j \langle 0^+_i || Q || 2^+_j \rangle \langle 2^+_j || Q || 0^+_i \rangle.
\]

\[
q_3(0^+_i) = \sqrt{\frac{7}{10}} \sum_{jk} \langle 0^+_i || Q || 2^+_j \rangle \langle 2^+_j || Q || 2^+_k \rangle \langle 2^+_k || Q || 0^+_i \rangle.
\]

Deformation parameters:

\[
q_2(0^+_i) = \left( \frac{3ZeR^2}{4\pi} \right)^2 \langle \beta^2 \rangle \equiv \left( \frac{3ZeR^2}{4\pi} \right)^2 \beta_{eff}^2
\]

\[
\frac{q_3(0^+_i)}{q_2^{3/2}(0^+_i)} = \frac{\langle \beta^3 \cos 3\gamma \rangle}{\langle \beta^2 \rangle^{3/2}} \equiv \cos 3\gamma_{eff}
\]

\[
R = r_0 A^{1/3}
\]

\[
r_0 = 1.2 \text{ fm}
\]
Global analysis of quadrupole shape invariants

Test of the 5DCHM quality:

FIG. 1. Theoretical excitation energies of the states $2^+_1$, $4^+_1$, $0^+_2$, $2^+_2$, and $2^+_3$ and the $B(E2; 0^+_1 \rightarrow 2^+_1)$ values (in ito of $e^2b^2$) in even-even nuclei, compared to the corresponding experimental values. The aim is not to compute properties of individual shape-coexisting nuclei, but to indicate mass regions that display structure properties associated with the phenomenon of shape coexistence. Based on the results obtained in the present analysis, we discuss the occurrence of shape coexistence in different regions of the table of nuclides.

(i) Nuclei in the vicinity of $Z \sim 50$ and $Z \sim 82$. The coexistence of low-lying spherical and intruder deformed shapes has been extensively studied and demonstrated by numerous experiments in Sn, Cd, Te, Pb, Hg, and Po isotopes. Shape coexistence in these regions can also be related to triaxiality, but the number of possible triaxial shape-coexisting nuclei is not large.

(ii) $Z \sim 64$ and $N \sim 90$ nuclei. The primary interest in this region is the rapid onset of deformation in the transition from $N = 86$ to $N = 92$. The issue of shape coexistence here is somewhat subtle because there are no obvious differences in band energy spacing or $B(E2)$ values. Moreover, the $0^+\_2$ states are found at relatively high energies because of strong mixing between the two lowest $K = 0$ bands.

(iii) $Z \sim 64$ and $N \sim 76$ nuclei. Medium-deformed triaxial ground states coexisting with highly deformed prolate excited state are predicted in this region. Furthermore, it is found that triaxial ground states originate from the interaction between proton multi-particle and neutron multi-hole states, and the prolate excited states are built on a deformed neutron shell gap with $\beta \sim 0.4$. This result is consistent with that obtained using the Gongy D1S effective interaction. New measurements of spectroscopic properties are suggested in this mass region, especially for the nuclei $^{134}$Nd, $^{136}$Sm, $^{140}$Gd, and $^{142}$Dy.

(iv) $Z \sim 40$ and $N \sim 60$ nuclei. The structure of nuclei in this mass region is characterized by a sudden onset of deformation in the transition from $N = 58$ to $N = 60$, as demonstrated by the dramatic change in the isotope shifts $\delta \langle r^2 \rangle$ and two-neutron separation energies $S_2^\text{nn}$. These changes occur because of the crossing between coexisting structures, that is, highly deformed prolate and spherical configurations. Numerous measurements of spectroscopic quadrupole moments, $B(E2)$ values, $E_{\text{trans}}$, and two-nucleon and $\alpha$-cluster transfer data, have revealed the onset of shape coexistence in Sr, Zr, and Mo isotopes, while data for static and dynamic quadrupole moments show that shape coexistence...
Global analysis of quadrupole shape invariants

- $Z \approx 64$ and $N \approx 76$: medium deformed triaxial ground state coexisting with highly deformed prolate excited state

\[
\frac{E(0^+_2)/E(2^+_1)}{E(0^+_2)/E(2^+_1)}
\]

\[
(a) |\beta_{\text{eff}} \cos 3\gamma_{\text{eff}} (0^+_2) - \beta_{\text{eff}} \cos 3\gamma_{\text{eff}} (0^+_1)|
\]

\[
(b) |\beta_{\text{eff}} (0^+_2) - \beta_{\text{eff}} (0^+_1)|
\]

Coexisting shapes in neutron-deficient Nd and Sm isotopes

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Linear response in deformed nuclei

- Implementation of the finite amplitude method for axially symmetric nuclei
- Alternative to the matrix formulation of the QRPA
- Avoids calculating the matrix elements of the residual interaction and diagonalizing large QRPA matrices
- Requires only moderate modifications of the existing ground state solvers
- The only cutoff is the size of the oscillator basis
- Enables large-scale calculations of the response function

\[
\begin{align*}
[E_\mu + E_\nu - \omega]X_{\mu\nu}(\omega) + \delta H^{20}_{\mu\nu}(\omega) &= -F^{20}_{\mu\nu} \\
[E_\mu + E_\nu + \omega]Y_{\mu\nu}(\omega) + \delta H^{02}_{\mu\nu}(\omega) &= -F^{02}_{\mu\nu}
\end{align*}
\]
Linear response in deformed nuclei

Preliminary results

- Isovector dipole strength in $^{144}\text{Sm}$, $^{148}\text{Sm}$ and $^{152}\text{Sm}$
Some other recent applications...

- ✔ Level of accuracy (rms deviation of experimental masses) of covariant EDFs is still below the state-of-the-art non-relativistic HFB mass models: additional terms should be included in the EDF – e.g. improving the effective mass

- ✔ Quantification of theoretical uncertainties within the EDF framework

- ✔ Is it possible to systematically reduce the number of parameters defining the EDF? ➔ Manifold boundary approximation method

- ✔ Description of fission dynamics (fission barriers, paths and lifetimes; induced fission dynamics

Work in progress
NEDFs provide an economic, global and accurate microscopic approach to nuclear structure that can be extended from relatively light systems to superheavy nuclei, and from the valley of $\beta$-stability to the particle drip-lines.

NEDF-based structure models that take into account collective correlations → microscopic description of low-energy observables: excitation spectra, transition rates, changes in masses, isotope and isomer shifts, related to shell evolution with nuclear deformation, angular momentum, and number of nucleons.

NEDF-based models are applicable to large-scale calculations.
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For more information please visit:
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