Mean-field and Beyond
Past, Present and Future

- Mean-field methods: what can and what cannot be calculated
- Applications and good reasons to go beyond mean-field
- How to do it (today)
- Applications

- The density functional theory: theorems

- Missing ingredients, new developments
- What remains to be done
Our group:

The precursors: P. Bonche, H. Flocard, M. Weiss, J. Dobaczewski

The successors: M. Bender, T. Duguet

Many collaborators: G. Bertsch, S. Cwiok, W. Nazarewicz, J. Skalski, P. Magierski…
Today:
the working tools

• Mean-field with effective interactions
• Typical applications
• First step beyond mean-field
  - symmetry restorations
  - configuration mixing
• Selected applications
Mean-field Methods

• Based on an “effective interaction” or a “density functional”
  The (small number of) parameters of the effective interaction
  are fixed by general considerations (no local adjustments)
• Pairing correlations are included at the BCS or better HFB level

• Full self-consistency
• No restrictions to a few shells, mean-field equations are solved
  as precisely as one wishes.
• Spherical and deformed nuclei are treated on the same footing,
  no “parametric deformation”
An example of an effective interaction: the Gogny force

It contains:
- A finite range central term:

$$V_C = \sum_{i=1,2} (V_W^i + V_M^i P^r + V_B^i P^\sigma + V_H^i P^\sigma P^r) \exp(-r^2/b_i^2)$$

- A zero range density dependent term

$$t_3(1 + x_3 P^\sigma)\rho(\vec{r})^\alpha$$

- Spin orbit and Coulomb

Parameters are adjusted on nuclear matter properties (saturation, ...) properties of a few magic nuclei
Mean-field energy curves ($\beta_2$ proportional to Q)
The competitors

Three families:

- **Gogny**: finite range including a density dependence, same interaction for HF and pairing
  (Bruyères le Chatel, Madrid, some Japanese groups)

- **Skyrme**: zero range, specific interaction for pairing, easy
  ("French group", "Polish group", P. Rheinardt et al., Japanese groups,…)

- **RMF**: relativistic but no exchange, pairing non relativistic
  (Munich-Zagreb, ….)
Skyrme HFB

$Q_\alpha$ for isotopic chains for super heavy elements (only even-even)

Cwiok, Heenen, Nazarewicz
Nature 2005
Skyrme HFB

Deformation properties of super-heavies
Beyond ground state properties of even-even nuclei

Breaking of time reversal invariance by a cranking constraint:

\[ H' = H - \omega J_x \]

rotational bands for deformed nuclei

by quasi particle excitations:
Odd nuclei : 1 qp states:
Even nuclei: 2qp states

Still a mean-field method
Full self-consistency for mean-field and pairing
Moments of inertia

Fig. 3. Kinematical (circles) and dynamical (diamonds) moment of inertia for $^{240}$Pu (top) and $^{244}$Pu (bottom). Open (filled) markers denote calculated (experimental) values.
Spectra of odd Z nuclei

![Diagram showing energy levels for nuclei 247Es, 251Md, and 255Lr.](image)
Plus and minus of the mean-field approach:

**Plus:**
- Starts from an effective interaction: generality
- Can describe any kind of shapes (from ground state to fission)
- Cranking (or qp excitations) well justified for deformed nuclei

**Minus:**
- Validity only for energy (variational) and one-body operators
- Breaking of symmetries (no direct determination of transitions)
- Soft nuclei? Shape coexistence?
- Effects of correlations beyond mean-field on masses?
Correlations

Explicitly included at the mean-field level:
• Statistics (fermions)
• Pairing (BCS or HFB)
• Deformation (can bring up to 20 MeV!)

Absent:
• Symmetry restoration
• Configuration mixing (shape, multi qp excitations, …)

Can all missing correlations be included in the interaction? ("DFT spirit")
Beyond mean-field

Set of mean-field wave functions depending on axial $q$

- Projection on $N$, $Z$, $J$:

  $$|J0q\rangle = \frac{1}{N_{J0q}} \hat{P}_Z \hat{P}_N |q\rangle,$$

- New wave functions by mixing on $q$:

  $$|J0k\rangle = \sum_q f_{J,k}(q) |J0q\rangle$$

with $f_{J,k}(q)$ determined by minimizing the energy:

$$E_{J,k} = \frac{\langle J0k | \hat{H} | J0k \rangle}{\langle J0k | J0k \rangle}$$
PLUS:
- Very rich basis with many ph components (more precisely qp excitations with respect to a spherical basis)
- GCM is not limited to small amplitude motion as the QRPA

MINUS:
- Kind of ph excitations determined by the constraint used in the mean-field
- Only time reversed pairs are excited
- Up to now, only axial states
Projection on angular momentum

= 

From intrinsic to laboratory frame of reference

No approximation based on the collective model for transition probabilities.
The spectroscopic quadrupole moment is given by:

\[
Q_c(J_k) = \sqrt{\frac{16\pi}{5}} \langle J, M = J, k|\hat{Q}_{20}|J, M = J, k \rangle \\
= \sqrt{\frac{16\pi}{5}} \frac{\langle J, J20|J,J \rangle}{\sqrt{2J+1}} \times \sum_{q,q'} f^*_{J,k}(q) f_{J,k}(q') \langle Jq||\hat{Q}_{20}||Jq' \rangle,
\]

Deformation parameters similar to collective ones have to be defined:

\[
\beta_2^{(s)}(J_k) = \sqrt{\frac{5}{16\pi}} \frac{4\pi Q_2^{(s)}(J_k)}{3R^2Z} \\
Q_2^{(s)}(J_k) = -\frac{2J+3}{J} Q_c(J_k)
\]

with \( R = 1.2 A^{1/3} \) and \( K = 0 \).
Mean field projected on J=0

Bars in red: 0\(^+\) states obtained after configuration mixing
Hartree-Fock + BCS (Skyrme SLy6 interaction + density dependent zero-range pairing force) \[\Rightarrow\] configuration mixing of angular-momentum and particle-number projected self-consistent mean field states

(M. Bender, P. Bonche, T. Duguet, and P.H. Heenen, PRC 69, 2004, 064303)

\[ ^{188}\text{Pb} \]

\[ \beta = 0.286(14) \]

\[ \beta = 0.30 \]
FIG. 14: Partial level scheme of $^{168}$Pb obtained by configuration mixing. The values of the B(E2) between all the states are given in Weisskopf units.
**Pb isotopic shifts**

**Fig. 3:** Difference from the experimental mean square charge radii (Expt), the beyond mean field calculations with normal [4] (MF) and decreased pairing [18] (MF*) and the IBM calculations (IBM) to the droplet model calculations for a spherical nucleus. Iso-deformation lines from the droplet model at $\beta_2 = 0.1$ and 0.15 are shown.
Collective wave functions
Global calculations

Correlations due to:
- symmetry restorations
- configuration mixing
Difference between exp and theory for masses

Red: with correlations
Two-proton gap for chains

Isotonic

Isotopic