Beyond the self-consistent mean-field:
Explicit treatment of shape fluctuations

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The Lead Radius Experiment
and Neutron Rich Matter in Astrophysics and in the Laboratory
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Physics goals of Multi-Reference Energy Density Functional calculations

- treat *dynamical* correlations not grasped by the *static* correlations in a symmetry-breaking single-reference (SR) Energy Density Functional (EDF) calculation, i.e. the fluctuations around the SR EDF minimum.

- treat *dynamical* correlations not easily absorbed into the EDF. Usually these are related to the finite size and surface of the system, strongly depend on the structure of the nucleus, and fluctuate rapidly with $N$, $Z$, deformation, . . .

- the correlations are not described by a *vertical* expansion in terms of np-nh excitations around the minimum, but by a *horizontal* expansion in terms of occupied states brought to the Fermi energy by the static correlations along a properly chosen collective path.

- move focus of EDF methods away from ground-state properties

- description of characteristic collective excited states at low excitation energy, hopefully also of states dominated by characteristic few-quasiparticle excitations (not yet tried in the EDF context)

- restore quantum numbers to have selection rules for transitions

- proper description of the transition from vibrational to rotational nuclei

- description of shape coexistence phenomena
Hypothesis: that there is a more-or-less clean and unique separation of correlations into three different classes

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2. Static correlations: deviation of a single deformed and paired mean-field state as described by a deformed and paired self-consistent mean-field ground state from a spherical Slater determinant
   - Correlated observables: multipole moments of the density, pairing gaps
   - Correlated excitations: rotational bands of well-deformed nuclei, 1- and 2-quasiparticle energies
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3. dynamical correlations: collective fluctuations around a given mean-field state described by a coherent superposition of many mean-field states
   - Correlated observables: out-of-band transition moments
   - Correlated excitations: vibrational states, rotational bands of not well-deformed nuclei
Symmetry restoration

particle-number projector

\[ \hat{P}_{N_0} = \frac{1}{2\pi} \int_0^{2\pi} \phi_N \, e^{-i\phi N_0} \, e^{i\phi N \hat{N}} \]

rotation in gauge space

angular-momentum restoration operator

\[ \hat{P}_{JM} = \frac{2J + 1}{16\pi^2} \int_0^{4\pi} \alpha \int_0^{\pi} \beta \sin(\beta) \int_0^{2\pi} \gamma \, D^*_M(\alpha, \beta, \gamma) \, \hat{R}(\alpha, \beta, \gamma) \]

rotation in real space

\( K \) is the z component of angular momentum in the body-fixed frame. Projected states are given by

\[ |JMq\rangle = \sum_{K=-J}^{+J} f_J(K) \, \hat{P}_{JM} \, \hat{P}^\dagger \, |q\rangle = \sum_{K=-J}^{+J} f_J(K) \, |JMlKlq\rangle \]

\( f_J(K) \) is the weight of the component \( K \) and determined variationally

Axial symmetry (with the z axis as symmetry axis) allows to perform the \( \alpha \) and \( \gamma \) integrations analytically, while the sum over \( K \) collapses, \( f_J(K) \sim \delta_{K0} \)
Superposition of angular-momentum projected SCMF states

\[ |JM\nu\rangle = \sum_q \sum_{K=-J}^{+J} f_{J\nu}(q, K) |JMqK\rangle \]

\[ \left\{ \begin{array}{l}
|JMqK\rangle \text{ projected mean-field state} \\
f_{J\nu}(q, K) \text{ weight function}
\end{array} \right. \]

\[ \frac{\delta}{\delta f_{J\nu}^*(q, K)} \frac{\langle JM\nu | \hat{H} | JM\nu \rangle}{\langle JM\nu | JM\nu \rangle} = 0 \quad \Rightarrow \quad \text{Hill-Wheeler-Griffin equation} \]

\[ \sum_{q'} \sum_{K'=-J}^{+J} \left[ \mathcal{H}_J(qK, q'K') - E_{J,\nu} \mathcal{I}_J(qK, q'K') \right] f_{J,\nu}(q'K') = 0 \]

with

\[ \mathcal{H}_J(qK, q'K') = \langle JMqK | \hat{H} | JMq'K' \rangle \quad \text{energy kernel} \]

\[ \mathcal{I}_J(qK, q'K') = \langle JMqK | JMq'K' \rangle \quad \text{norm kernel} \]

A Hamiltonian is used here for the transparent formulation of the principles of projection and the GCM. The actual calculations use an energy density functional, in what should be called *multi-reference energy density functional* (MR EDF) calculations.
The angular-momentum projected GCM gives the
- correlated ground state for each value of $J$
- spectrum of excited states for each $J$
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A few more technical points

- the weight functions $f_{J,\nu}(q, K)$ are not orthonormal
- orthonormal wave functions $g_{J,\nu}(q, K)$ can be constructed as
  $$ g_{J,\nu}(q, K) = \sum_{q'} \sum_{K'} \mathcal{I}_{\frac{1}{2}}(q, k; q', K') f_{J,\nu}(q', K') $$

- $|g_{J,\nu}(q, K)|^2$ is not the probability to find the projected mean-field state $|JMqK\rangle$ in the GCM state $|J\nu K\rangle$, as the $|JMqK\rangle$ do not form a orthogonal basis
- projection is a special case of the GCM, where the group structure determines the collective path and the weight function.
- angular momentum-projection is part of the “quadrupole correlations”, as it mixes states with different orientations of the quadrupole tensor.
- projected GCM is not a Bohr-Hamiltonian! There is neither a collective potential energy surface nor explicit mass parameters
Typical Situations

\[ E \text{ (MeV)} \]

- $^{208}\text{Pb}$
- $^{180}\text{Hg}$
- $^{202}\text{Rn}$
- $^{170}\text{Hf}$

\[ g_{gs} \]

- $\beta_2$


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$E$ (MeV) vs. $\beta_2$


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Configuration mixing via the projected Generator Coordinate Method

Configuration mixing via the projected Generator Coordinate Method

Transition moments


- in-band and out-of-band $E2$ transition moments directly in the laboratory frame with correct selection rules
- full model space of occupied particles
- only occupied single-particle states contribute to the kernels ("horizontal expansion")
- $\Rightarrow$ no effective charges necessary
- no adjustable parameters

\[
B(E2; J'_\nu \rightarrow J_\nu) = \frac{e^2}{2J' + 1} \sum_{M=-J}^{+J} \sum_{M'=-J'}^{+J'} \sum_{\mu=-2}^{+2} |\langle JM\nu | \hat{Q}_{2\mu} | J'_M \nu' \rangle|^2
\]

\[
\beta_2^{(t)} = \frac{4\pi}{3R^2A} \sqrt{\frac{B(E2; J \rightarrow J - 2)}{(J \ 0 \ 2 \ 0 | (J - 2) \ 0)^2 e^2}} \ \text{with} \ R = 1.2 A^{1/3}
\]
Masses from self-consistent mean-field calculations

- Skyrme interaction SLy4 + density-dependent pairing interaction
- other parameterizations give qualitatively similar results
- Wrong trend with $A$
- overestimated shell effects visible at $N = 20, 50, 82$ and $126$
- missing Wigner energy
- The slightly wrong trend with mass and isospin can be removed by a slight (a few permille) perturbative readjustment of the parameters of SLy4. The major change is a reduction of the volume energy coefficient by 0.09 MeV.
- And what about the arches?
Static and Dynamic Quadrupole Correlation Energies


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Beyond the self-consistent mean-field

![Graph showing dynamical correlation energy vs Neutron Number and Proton Number]
Static and Dynamic Quadrupole Correlation Energies


Beyond the self-consistent mean-field
Intrinsic Deformation and Quadrupole Correlation Energy


Beyond the self-consistent mean-field
Eigenvalues of the single-particle Hamiltonian vs. $S_{2q}$

lower panel: $-S_{2p}(Z=50, N)/2$
The global linear trend is taken out subtracting $\frac{N-82}{2}[S_{2p}(Z=50, N=50) - S_{2p}(Z=50, N=82)]$
using the spherical mean-field $S_{2p}$


lower panel: $-S_{2n}(Z, N=50)/2$
The global linear trend is taken out subtracting $\frac{N-50}{2}[S_{2n}(Z=28, N=50) - S_{2n}(Z=50, N=50)]$
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Beyond the self-consistent mean-field
Two-nucleon gaps

\[ \delta_{2p}(N, Z) = S_{2p}(Z, N) - S_{2p}(Z - 2, N) \]

\[ \delta_{2n}(N, Z) = S_{2n}(Z, N) - S_{2n}(Z, N - 2) \]

experimental values include more recent data than the plots in the papers
Collectivity-enhanced quenching of signatures of shell closures
Collectivity-enhanced quenching of signatures of shell closures

Effect of shape fluctuations on rms charge radii

Beyond the self-consistent mean-field
Effect of shape fluctuations on rms charge radii


Beyond the self-consistent mean-field
Effect of shape fluctuations on rms charge radii


Beyond the self-consistent mean-field
Effect of shape fluctuations on neutron skins

M. B., G. F. Bertsch, P.-H. Heenen, unpublished material

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Beyond the self-consistent mean-field
More specifically: $^{208}\text{Pb}$

<table>
<thead>
<tr>
<th></th>
<th>$r_p$</th>
<th>$r_n$</th>
<th>skin</th>
</tr>
</thead>
<tbody>
<tr>
<td>HF spherical</td>
<td>5.451</td>
<td>5.608</td>
<td>0.157</td>
</tr>
<tr>
<td>HF+BCS spherical</td>
<td>5.453</td>
<td>5.610</td>
<td>0.157</td>
</tr>
<tr>
<td>minimum $J=0$</td>
<td>5.460</td>
<td>5.617</td>
<td>0.157</td>
</tr>
<tr>
<td>GCM</td>
<td>5.459</td>
<td>5.616</td>
<td>0.157</td>
</tr>
</tbody>
</table>

The rms radii shown are those of point particles in fm.
Other degrees of freedom: triaxiality, octupole, pairing

- Projection on angular momentum and mixing of states with non-axial shapes
- Octupole deformation $\beta_3$
- Projection on parity $\pm 1$
- Mixing of states with different $\beta_3$
- Particle-number projection using physical pairing strength $V_0$
- Mixing of states generated varying the mean-field neutron pairing strength $V_n$ (↔ constraint on amount of pairing correlations)

M. B., T. Duguet, IJMPE 16 (2007) 222
Outlook: Questions to be addressed and answered

- problems with collective states in MR-EDF calculations suggest that there is an urgent need for **improved parameterizations** of the nuclear energy density functional that give better single-particle spectra. Which are the relevant terms in the functional, how to adjust them to which observables? (the tensor interaction is *not* an important missing piece)

- How to define a suitable and exhaustive **collective space** for MR-EDF calculations? The systematically too dilute excitation spectra suggest that the current collective space misses degrees of freedom important for the "moments of inertia" (to have "Thouless-Valatin" instead of "Peierls-Yoccoz"). Which symmetries to break, which to restore, how many collective degrees of freedom to take into account, how to optimize the collective path/surface, how to take single-particle degrees of freedom into account, without sacrificing the applicability of the method to all nuclei (with computers available at the time this has been worked out)?

- A **formal framework** for MR-EDF calculations has be be established to avoid surprises from spurious contributions to the energy density functional when using clever tricks originally invented for operators (D. Lacroix, T. Duguet, M. B., *et al.*, arxiv:0809.2041v2, arxiv:0809.2045v2, arxiv:0809.2049v2, all Phys. Rev. C, in press)
The work presented here would have been impossible without my collaborators on the various subjects touched upon during this talk.

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