Mass models based on self-consistent mean fields Role of explicit correlations

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Overview

Our long-term goal:

- universal microscopic model for characteristic low-lying states of nuclei ...
- ... and large-amplitude dynamics of nuclei ...
- ... irrespective of their mass and N Z ...
- ... their having even or odd N or Z ...
- ... using a universal effective interaction / energy density functional.

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Methodology:

- Single-reference: nearly symmetry-unrestricted self-consistent mean-fields ("static" deformation and pairing correlations through symmetry breaking)
- Multi-reference: symmetry restoration
- Multi-reference: configuration mixing by the Generator Coordinate Method (GCM)

("dynamical" deformation and pairing correlations)

- Skyrme contact interactions (or energy density functional) + Coulomb
- for most results shown: parametrization SLy4 which is not a mass model, but an effective interaction for nuclear structure, response and dynamics – (10 parameters) + density-dependent pairing interaction (2 parameters + cutoff)
- coordinate-space representation in a 3d box using Lagrange-mesh techniques Baye & Heenen, PRC 29 (1984) 1056; JPA 19 (1986) 2041
 - no difficulty to converge the exponential tail of the wave function
 - convergence in terms of step size is practically independent on the deformation and N/Z ratio
- at time being: axial or triaxial reflection-symmetric shapes
- pairing treated in a Bogoliubov-type approach
- constraints on quadrupole deformations and/or one component of angular momentum

configuration constraints ("blocking")

- 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

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- move focus of EDF methods away from ground-state properties
- description of characteristic excited states at low excitation energy
- restore quantum numbers to have selection rules for transitions
- description of the transition from vibrational to rotational nuclei
- description of shape coexistence phenomena

particle-number projector



angular-momentum restoration operator

rotation in real space

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

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

$$|JMq\rangle = \sum_{K=-J}^{+J} f_J(K) \hat{P}^J_{MK} \hat{P}^Z \hat{P}^N |q\rangle = \sum_{K=-J}^{+J} f_J(K) |JMKq\rangle$$

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

Axial symmetry (with the z axis as symmetry axis) allows to perform the α and γ integrations analytically, while the sum over K collapses, $f_J(K) \sim \delta_{K0}$



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Configuration mixing by the symmetry-restored Generator Coordinate $\ensuremath{\mathsf{Method}}$

Superposition of projected self-consistent mean-field states $|\mathsf{MF}(q)\rangle$ differing in some collective coordinate(s) q

$$|NZJM\nu\rangle = \sum_{q} \sum_{K=-J}^{+J} f_{J,K}^{NZ}(q,K) \hat{P}_{MK}^{J} \hat{P}^{Z} \hat{P}^{N} |\mathsf{MF}(q)\rangle = \sum_{q} \sum_{K=-J}^{+J} f_{J\nu}^{NZ}(q,K) |NZ JM qK\rangle$$

with weights $f_{J\nu}^{NZ}(q,K)$.

$$\frac{\delta}{\delta f_{J\nu}^{*}(q,K)} \frac{\langle NZ JM\nu | \hat{H} | NZ JM\nu \rangle}{\langle NZ JM\nu | NZ JM\nu \rangle} = 0 \quad \Rightarrow \quad \text{Hill-Wheeler-Griffin equation}$$
$$\sum_{q'} \sum_{K'=-J}^{+J} \left[\mathcal{H}_{J}^{NZ}(qK,q'K') - E_{J,\nu}^{NZ} \mathcal{I}_{J}^{NZ}(qK,q'K') \right] f_{J,\nu}^{NZ}(q'K') = 0$$

with

 $\begin{array}{l} \mathcal{H}_{J}(qK,q'K') = \langle NZ \; JM \; qK | \hat{H} | NZ \; JM \; q'K' \rangle & \text{energy kernel} \\ \mathcal{I}_{J}(qK,q'K') = \langle NZ \; JM \; qK | NZ \; JM \; q'K' \rangle & \text{norm kernel} \end{array}$

Angular-momentum projected GCM gives the

- \blacktriangleright correlated ground state for each value of J
- spectrum of excited states for each J

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Other typical situations





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G. F. Bertsch, B. Sabbey, M. Uusnäkki, Phys. Rev. C 71 (2005) 054311.



- 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.
- But what about the arches?

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503.



Intrinsic Deformation and Quadrupole Correlation Energy



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

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Mass residuals

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M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322

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Mass residuals



- Shell effects are not overestimated in general, they are overestimated for neutrons
- This might well be a problem with the effective interaction, not so much with large missing correlations

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322



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M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

How is the evolution of shell structure related to systematics of masses?

PRL 101, 052502 (2008) PHYSICAL REVIEW LETTERS week ending 1 AUGUST 2008

Evolution of the N = 50 Shell Gap Energy towards ⁷⁸Ni

J. Hakala, S. Rahaman, V.-V. Elomaa, T. Eronen, U. Hager,* A. Jokinen, A. Kankainen, I. D. Moore, H. Penttilä,

S. Rinta-Antila,[†] J. Rissanen, A. Saastamoinen, T. Sonoda,[‡] C. Weber, and J. Ävstö[§]

Department of Physics, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland (Received 20 March 2008; published 31 July 2008)



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

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} M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

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

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$$\begin{aligned} \delta_{2p}(N,Z) &= S_{2p}(Z,N) - S_{2p}(Z-2,N) \\ \delta_{2n}(N,Z) &= S_{2n}(Z,N) - S_{2n}(Z,N-2) \end{aligned}$$

In spite of their name, the two-nucleon shell gaps do not measure the gap in the single-particle spectrum in self-consistent mean-field model

M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102505 M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. C 73 (2006) 034322 experimental values shown here include more recent data than the plots in the papers



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M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

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Collectivity-enhanced quenching of signatures of shell closures

(a) (b) HFB 3 () 40 30 0 20 162 S_{2N} (MeV) 20 5DCH 5DCF 3 () 30 0 20 S_{2N} (MeV) 20 EXP EXP 30 (MeV) 20 № 8 00 gw (MeV) 20 sc (MeV) 10 10 Λ 120 140 160 180 200 J.-P. Delaroche, M. Girod, J. Libert, H. Goutte, S. Hilaire, S. Péru, N. Pillet, G. F. Bertsch, PRC81 (2010) 014303

same effect seen in 5-dimensional collective Hamiltonian from Gogny D1s





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filled symbols: all nuclei in the sample open symbols: nuclei with N, Z > 30

M. B., G. F. Bertsch, P.-H. Heenen, PRC 78 (2008) 054312

RMS residuals of the binding energy and various

Theory	Е	S _{2n}	S_{2p}	δ_{2n}
spherical SCMF	11.7	1.6	1.6	1.2
deformed SCMF	5.3	1.1	1.0	1.2
+ J = 0	4.4	0.9	0.8	0.9
+ GCM	4.4	0.8	0.8	0.8

Same as above but for heavy nuclei with N, Z > 30 only (i.e. excluding the ones affected by Wigner energy)

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Theory	Ε	S _{2n}	S_{2p}	δ_{2n}
spherical SCMF	12.6	1.6	1.5	0.9
deformed SCMF	5.5	0.9	0.6	0.9
+ J = 0	3.9	0.8	0.5	0.7
+ GCM	3.8	0.7	0.5	0.5

... and these numbers are for the non-corrected SLy4.



M. B., G. F. Bertsch, P.-H. Heenen, Phys. Rev. Lett. 94 (2005) 102503.

Role of correlations for transactinide nuclei



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M. B.and P.-H. Heenen, to be published

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Other degrees of freedom: octupole and pairing



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Limitations of the existing implementations of the method

- limited to even-even nuclei
- collective states only
- excitation spectra too spread out

What is the missing physics?

explicit coupling to single-particle degrees of freedom

How to introduce the missing physics?

- Use HFB states breaking intrinsic time-reversal invariance as basis states for the projected GCM
- cranked HFB states describe the alignment of single-particle states with the rotation axis and the weakening of pairing with increasing J

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- blocked HFB states describe single-particle excitations (K isomers in even-even nuclei, odd-A nuclei, odd-odd nuclei)
- + adjustment of improved energy functionals

There was a formal problem to be understood first

- All standard energy density functionals (EDF) used for mean-field models and beyond do not correspond to the expectation value of a Hamiltonian for at least one of the following reasons:
 - density dependences
 - the use of different effective interactions in the particle-hole and pairing parts of the energy functional
 - the omission, approximation or modification of specific exchange terms

that are all introduced for phenomenological reasons and/or the sake of numerical efficiency.

- consequence: breaking of the exchange symmetry under particle exchange when calculating the energy, leading to non-physical interactions of a given nucleon or pair of nucleons with itself
- > these self-interactions remain (usually) hidden in the mean field
- ▶ in the extension to symmetry-restored GCM, these terms cause
 - discontinuities and divergences in symmetry-restored energy surfaces
 - breaking of sum rules in symmetry restoration
 - potentially multi-valued EDF in case of standard density-dependencies

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Anguiano, Egido, Robledo NPA696 (2001) 467 Dobaczewski, Stoitsov, Nazarewicz, Reinhard, PRC 76 (2007) 054315 Lacroix, Duguet, Bender, PRC 79 (2009) 044318 Bender, Duguet, Lacroix, PRC 79 (2009) 044319 Duguet, Bender, Bennaceur, Lacroix, Lesinski, PRC 79 (2009) 044320 Bender, Avez, Duguet, Heenen, Lacroix, in preparation constructing the EDF as expectation value of a strict Hamiltonian. Problems: numerically very costly due to Coulomb exchange & pairing. no

available parameterizations of reasonable quality (the difficulties to construct such parametrizations was the main motivation to use EDFs in the 1970s).

- 2. construct the EDF from a density-dependent Hamiltonians with special treatment of the density entering density dependent terms for which high-quality parameterizations can be constructed. Problems: numerically very costly due to Coulomb exchange & pairing; cannot be defined for all possible confifuration mixing [Robledo, JPG 37 (2010) 064020].
- 3. introduce a regularization scheme of the EDF

that allows for the use of (almost) standard functionals [Lacroix, Duguet, & Bender, PRC 79 (2009) 044318] for which numerically efficient high-quality parameterizations can be easily constructed [Washiyama, Bennaceur, Avez, Bender, Heenen, & Hellemans, PRC 86 (2012) 054309]. Problems: complicated formalism; does not remove all internal inconsistencies.

How to construct a suitable Hamiltonian?

- many-body forces instead of density dependences
- there no existing parametrization that gives simultaneously
 - realistic "standard" nuclear matter properties
 - repulsive spin-spin interaction
 - attractive pairing

which was the reason to introduce density dependences etc. in the 1970s.

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The caricature of a contact Hamiltonian: SLyMR0

$$\begin{split} \hat{\nu} &= t_0 \left(1 + x_0 \hat{P}_{\sigma} \right) \hat{\delta}_{r_1 r_2} \\ &+ \frac{t_1}{2} \left(1 + x_1 \hat{P}_{\sigma} \right) \left(\hat{\mathbf{k}}_{12}^{\,\prime 2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12}^{\,2} \right) \\ &+ t_2 \left(1 + x_2 \hat{P}_{\sigma} \right) \hat{\mathbf{k}}_{12}^{\,\prime 2} \cdot \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\ &+ \mathrm{i} \, W_0 \left(\hat{\boldsymbol{\sigma}}_1 + \hat{\boldsymbol{\sigma}}_2 \right) \cdot \hat{\mathbf{k}}_{12}^{\,\prime} \times \hat{\delta}_{r_1 r_2} \hat{\mathbf{k}}_{12} \\ &+ u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \right) \\ &+ v_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4} + \hat{\delta}_{r_1 r_2} \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_2 r_4} + \cdots \right) \end{split}$$

J. Sadoudi, M. Bender, K. Bennaceur, D. Davesne, R. Jodon, and T. Duguet, Physica Scripta T, in press

Energy surfaces

HFB ground state projected on





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HFB state cranked to $\langle J_z \rangle = 2$ projected on



N = Z = 12

B. Avez, B. Bally, M. B., P.-H. Heenen (to be published)

Decomposition



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Odd-A nuclei with SLyMR0: The example of ^{25}Mg

B. Bally, B. Avez, M. B., P.-H. Heenen (to be published)



HFB ground state with $\langle \hat{N} \rangle = 13, \langle \hat{Z} \rangle = 12$)

"False vacuum" (non-blocked Blocked HFB 1-quasiparticle state, where blocked particle has $\langle j_z \rangle \approx 5/2$

Blocked HFB 1-quasiparticle state, where blocked particle has $\langle j_z \rangle \approx 3/2$



B. Bally, B. Avez, M. B., P.-H. Heenen (to be published)



Most general central 3-body contact force with two gradients

$$\begin{split} \hat{\mathbf{v}}_{123} &= \mathbf{u}_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \right) \\ &+ \frac{\mathbf{u}_1}{2} \left[1 + y_1 P_{12}^{\sigma} \right] \left(\hat{\mathbf{k}}_{12} \cdot \hat{\mathbf{k}}_{12} + \hat{\mathbf{k}}_{12}' \cdot \hat{\mathbf{k}}_{12}' \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\ &+ \frac{\mathbf{u}_1}{2} \left[1 + y_1 P_{31}^{\sigma} \right] \left(\hat{\mathbf{k}}_{31} \cdot \hat{\mathbf{k}}_{31} + \hat{\mathbf{k}}_{31}' \cdot \hat{\mathbf{k}}_{31}' \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\ &+ \frac{\mathbf{u}_1}{2} \left[1 + y_1 P_{23}^{\sigma} \right] \left(\hat{\mathbf{k}}_{23} \cdot \hat{\mathbf{k}}_{23} + \hat{\mathbf{k}}_{23}' \cdot \hat{\mathbf{k}}_{23}' \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \\ &+ \mathbf{u}_2 \left[1 + y_{21} P_{12}^{\sigma} + y_{22} (P_{13}^{\sigma} + P_{23}^{\sigma}) \right] \left(\hat{\mathbf{k}}_{12} \cdot \hat{\mathbf{k}}_{12}' \right) \hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \\ &+ \mathbf{u}_2 \left[1 + y_{21} P_{31}^{\sigma} + y_{22} (P_{32}^{\sigma} + P_{12}^{\sigma}) \right] \left(\hat{\mathbf{k}}_{31} \cdot \hat{\mathbf{k}}_{31}' \right) \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_2} \\ &+ \mathbf{u}_2 \left[1 + y_{21} P_{23}^{\sigma} + y_{22} (P_{21}^{\sigma} + P_{31}^{\sigma}) \right] \left(\hat{\mathbf{k}}_{23} \cdot \hat{\mathbf{k}}_{23}' \right) \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \end{split}$$

J. Sadoudi, T. Duguet, M. B., J. Meyer (to be published)

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- Within EDF-based models, correlations from shape fluctuations and symmetry can have a large impact on binding energy differences around (spherical) shell closures
- in EDF-based models, there is a collectivity enhanced quenching of the separation energies at mid-shell that has to be distinguished from "real quenching" of the gaps in the spectrum of eigenvalues of the spherical single-particle Hamiltonian
- most parametrizations of EDF methods describe proton mass differences across proton shell closures much better than across neutron shell closures
- systematics of radii slightly improve when adding dynamical correlations, which is a consistency check of the collective ground-state wave functions
- while dynamical correlations always increase masses (of even-even nuclei) (properties of projectors, variational principle), they might reduce radii in some particular cases
- for all models and/or parametrizations, some regions in the nuclear chart are better described than others

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Outlook

Do we need

- more correlations?
- higher-order terms in the effective interaction / functional?
- connection to *ab-initio* methods?
- better fit protocols?
- ▶ ...?

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Developments under way (in my collaboration)

- Generalization to angular-momentum-optimized reference states
 - improved moments of inertia
 - modeling of K isomers
 - modeling of odd-A nuclei (and eventually odd-odd nuclei)
- benchmarking of efficient approximations to full calculations
- Construction of suitable Hamiltonians to replace more general functionals (3-body forces with gradients, higher-order gradient terms, ...)

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But what about

- reflection asymmetric shapes (octupole, cluster states, ...)
- isospin restoration (Wigner energy?)
- projection before variation

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The collaboration

- B. Avez, B. Bally, M. Bender, J. Sadoudi CEN Bordeaux Gradignan, France formalism; beyond-mean-field models; construction of effective interactions; applications to complex nuclei
- K. Bennaceur, D. Davesne, R. Jodon, J. Meyer IPN Lyon, France construction of effective interactions; parameter fit; nuclear matter
- T. Duguet SPhN / Irfu / CEA Saclay, France formalism; construction of effective interactions
- P.-H. Heenen, V. Hellemans, W. Ryssen Université Libre de Bruxelles, Belgium beyond-mean-field models, applications to complex nuclei

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