Beyond Mean-Field Calculations for Odd-Mass Nuclei

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Semantic Intermezzo

- EDF: Energy Density Functional

- SR-EDF: Single-Reference EDF
  $\approx$ Mean-field, HFB, nuclear DFT, ...

- MR-EDF: Multi-Reference EDF
  $\approx$ Beyond-mean-field, Projected GCM, ...

Outline of the EDF method

1. Nuclear binding energy: $\mathcal{E}^{nuc}[\rho, \kappa, \kappa^*]$
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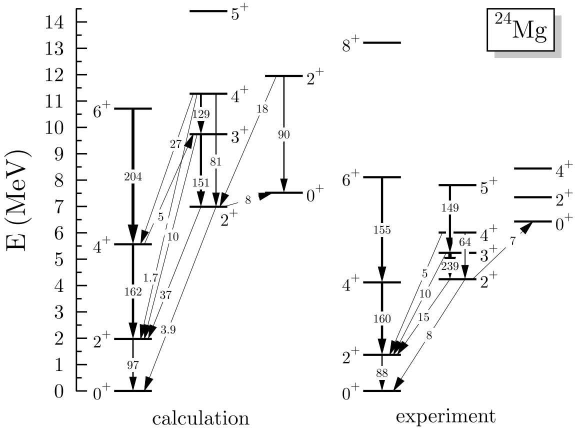
Goals of the PhD

- Example for even-evenu nuclei:
  Bender, Heenen, PRC **78** 024309 (2008)



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Possibilities:

- Similar level of modeling in the description of even-even and odd-even nuclei in the EDF method.
- Spectroscopy of odd-even nuclei.
  Observables: angular momentum, parity, excitation energies, moments, transition probabilites, ...

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Required:

- Configuration mixing of particle-number and angular-momentum projected one-quasiparticle states.

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Energy functional

$$\mathcal{E}^{nuc}[\rho, \kappa, \kappa^*]^{ab} = \frac{\langle \Phi_a | \hat{H} | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle}$$

$$\rho^{ab} = \frac{\langle \Phi_a | \hat{a}^\dagger \hat{a} | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle}, \quad \kappa^{ab} = \frac{\langle \Phi_a | \hat{a} \hat{a} | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle}, \quad \kappa_t^{ba\,*} = \frac{\langle \Phi_a | \hat{a}^\dagger \hat{a}^\dagger | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle}.$$

- $|\Phi_a\rangle$, $|\Phi_b\rangle$: different quasiparticle states.
  $\langle \Phi_a | \Phi_b \rangle \neq 0$ (condition to use the EWT of Balian-Brézin)

- $\mathcal{E}^{nuc}$ **directly and uniquely** determined by $\hat{H}$.
  $\Rightarrow$ respect the **Pauli principle**.

What's in $\hat{H}$?

$$\hat{H} = \hat{K}^{(1)} + \hat{V}^{(2)}_{Coul} + \hat{V}^{(2\text{-}4)}_{Sky}$$

- $\hat{K}^{(1)}$: kinetic energy (+ CoM corr.).
- $\hat{V}^{(2)}_{Coul}$: Coulomb interaction.
- $\hat{V}^{(2\text{-}4)}_{Sky}$: Skyrme pseudo-potential. **Phenomenological**.

The Skyrme pseudo-potential

$$\hat{V}^{(2\text{-}4)}_{Sky} = \hat{V}^{(2)}_{Sky} + \hat{V}^{(3)}_{Sky} + \hat{V}^{(4)}_{Sky}$$

- $\hat{V}^{(2)}_{Sky} = t_0 \left(1 + x_0 \hat{\Gamma}^{\sigma}_{12}\right) \hat{\delta}_{r_1 r_2} + \frac{t_1}{2} \left(1 + x_1 \hat{\Gamma}^{\sigma}_{12}\right) \left(\hat{\vec{k}}'^{2}_{12}\, \hat{\delta}_{r_1 r_2} + \hat{\delta}_{r_1 r_2}\, \hat{\vec{k}}^{2}_{12} \right) +$
  $t_2 \left(1 + x_2 \hat{\Gamma}^{\sigma}_{12}\right) \hat{\vec{k}}'_{12}\, \hat{\delta}_{r_1 r_2} \cdot \hat{\vec{k}}_{12} + i W_0 \left(\hat{\vec{\sigma}}_1 + \hat{\vec{\sigma}}_2\right) \hat{\vec{k}}'_{12}\, \hat{\delta}_{r_1 r_2} \times \hat{\vec{k}}_{12}$
- $\hat{V}^{(3)}_{Sky} = u_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} + \hat{\delta}_{r_3 r_2} \hat{\delta}_{r_1 r_3} + \hat{\delta}_{r_2 r_1} \hat{\delta}_{r_3 r_1} \right)$
- $\hat{V}^{(4)}_{Sky} = v_0 \left(\hat{\delta}_{r_1 r_3} \hat{\delta}_{r_2 r_3} \hat{\delta}_{r_3 r_4} + \ldots \right)$
- **9** parameters.

- SLyMR0 parametrization.
  Sadoudi *et al.* Physica Scripta T154 014013 (2013).

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Bogoliubov quasiparticle states

- Defined by a unitary Bogoliubov transformation.
- Generalized product states (Slater determinants).
- Include **pairing** correlations
  ... but do not have a good number of particles.
- We restrict ourselves to the symmetries of a subgroup of D_{2h}^{TD} (parity, signature, y-time Simplex).
  $\Rightarrow$ **Triaxial deformations**.
- We consider only **one-quasiparticle** excitations.

Minimization of quasiparticle states

Minimization: $\delta\mathcal{E}^{nuc}[\rho,\kappa,\kappa^*]^{aa} = 0$

Constraints using Lagrange parameters:

- Neutron number: $\langle\Phi_a|\hat{N}|\Phi_a\rangle = N$
- Proton number: $\langle\Phi_a|\hat{Z}|\Phi_a\rangle = Z$
- Quadrupole deformation: $\langle\Phi_a|\hat{Q}|\Phi_a\rangle = Q$

Minimization of quasiparticle states

Minimization: $\delta\mathcal{E}^{nuc}[\rho,\kappa,\kappa^*]^{aa} = 0$

- Self-consistent problem: solved by an iterative procedure.
- Solved on a 3d cartesian mesh.

- Solved for different values of Q and/or one-quasiparticle excitations.

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Symmetry group of the Hamiltonian

Let G be a group with an unitary representation: $g \in G \to \hat{U}(g)$ and irreducible representations $D^{\lambda}(G)$ of dimension d_{λ}.

Symmetry group of the Hamiltonian

$$\forall\, g \in G\,,\ [\hat{H}, \hat{U}(g)] = 0$$

Consequences:

- There exist common bases for the eigenspaces of $\hat{H}$ and the irreps $D^{\lambda}(G)$ of $G \Rightarrow$ quantum number λ
- The eigenstates of $\hat{H}$ have degeneracies $\geq d_{\lambda}$.

Symmetry broken by the quasiparticle states

The quasiparticle state $|\Phi_a\rangle$ breaks the symmetry G of the Hamiltonian:

$$|\Phi_a\rangle = \sum_{\lambda} \sum_{\tau} \sum_{i=1}^{d_\lambda} c_i^{\lambda\tau} \, |\lambda i \tau, a\rangle$$

$|\lambda i \tau, a\rangle$: basis state of $D^\lambda(G)$ in the subspace $S(G|\Phi_a\rangle)$

$S(G|\Phi_a\rangle) \equiv \{ \displaystyle\oint f(g)\, \hat{U}(g)|\Phi_a\rangle,\, f(g) \in L^2(G) \}$

This is contrary to the properties of the eigenstates of $\hat{H}$ (but this is simpler at the SR-EDF level).

Projection Operators

Projection operator $\hat{P}^{\nu}_{lm}$:

$$\hat{P}^{\nu}_{lm}|\lambda i\rangle = \delta_{\nu\lambda}\,\delta_{mi}\,|\lambda l\rangle$$

Properties:

$$\hat{P}^{\nu}_{lm}{}^{\dagger} = \hat{P}^{\nu}_{ml}$$

$$\hat{P}^{\nu}_{jk}\,\hat{P}^{\mu}_{lm} = \hat{P}^{\nu}_{jm}\,\delta_{\nu\mu}\delta_{kl}$$

Finite groups:

$$\hat{P}^{\nu}_{lm} = \frac{d_\nu}{n_G}\sum_{g}^{n_G} D^{\nu}_{lm}{}^{*}(g)\,\hat{U}(g)$$

Compact Lie groups:

$$\hat{P}^{\nu}_{lm} = \frac{d_\nu}{v_G}\int_{g\in G} dv_G(g)\,D^{\nu}_{lm}{}^{*}(g)\,\hat{U}(g)$$

Symmetry restoration by a projection technique

Projection of a quasiparticle state

$$\hat{P}^{\nu}_{lm}|\Phi_a\rangle = \sum_{\tau} c^{\nu\tau}_{m} \, |\nu l \tau, a\rangle$$

Sufficient for abelian groups ($d_\nu = 1$), otherwise we have also to diagonalize $\hat{H}$:

$$|\nu \, l \, \epsilon, a\rangle = \sum_{m=1}^{d_\nu} f^{\nu}_{\epsilon}(a, m) \, \hat{P}^{\nu}_{lm}|\Phi_a\rangle$$

$$\frac{\delta}{\delta f^{\nu *}_{\epsilon}(a, m')} \left(\frac{\langle \nu l \epsilon, a|\hat{H}|\nu l \epsilon, a\rangle}{\langle \nu l \epsilon, a|\nu l \epsilon, a\rangle} \right) = 0$$

Particle-number and angular-momentum projections

Conservation of the neutron and proton numbers:

- $U(1)_N \times U(1)_Z$
- Broken by: pairing correlations.

Conservation of total angular momentum:

- $SU(2)_A$
- Broken by: quadrupole deformation.

Configuration mixing (GCM)

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Congiguration mixing

- Mixing of projected states obtained from different quasiparticle states $(|\Phi_a\rangle, |\Phi_b\rangle, \dots)$.

Configuration mixing (GCM)

- $|\Lambda M \xi\rangle = \sum_{i=1}^{\Omega_I} \sum_{\epsilon=1}^{\Omega_i^\Lambda} F_\xi^\Lambda(i,\epsilon) |\Lambda M \epsilon, i\rangle$

  $\Lambda \equiv (J, N, Z, P)$
  Ω_I : set of states $|\Phi_i\rangle$
  Ω_i^Λ : set of projected states given (Λ, i).

- i : deformation and blocked quasiparticle.

$$\frac{\delta}{\delta F_\xi^{\Lambda *}(i,\epsilon)} \left(\frac{\langle \Lambda M \xi | \hat{H} | \Lambda M \xi \rangle}{\langle \Lambda M \xi | \Lambda M \xi \rangle} \right) = 0 \Longrightarrow F_\xi^\Lambda(i,\epsilon) \text{ et } E_\xi^\Lambda(\Omega_I)$$

Outline of the EDF method v2.0

We define a EDF ($\equiv$ effective Hamiltonian).

$\downarrow$

We create a set of one-quasiparticle states: $|\Phi_a\rangle$, $(a = \ldots)$.

$\downarrow$

We project each of them on the good quantum numbers: $|JMNZP\epsilon, a\rangle$.

$\downarrow$

We diagonalize the (effective) Hamiltonian between the projected states: $|JMNZP\xi\rangle$.

$\downarrow$

We calculate observables.

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Motivations

- Proof of principle.
- Light nucleus with a simple structure.
- Phys. Rev. Lett. **113** 162501 (2014)

Parallel computational resources

CNRS-GENCI

Supercomputer **Turing**

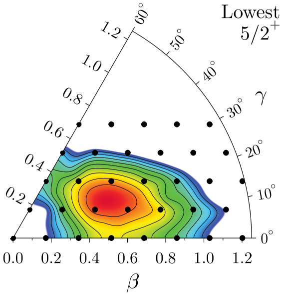
- 838.9 Teraflops.
- ≈ 600 000 CPU hours (≈ 345 million hours available/year).

University of Bordeaux

Supercomputer **Avakas**

- 38.8 Teraflops.
- ≈ 200 000 Turing equivalent hours.

Characteristics of the Configuration Mixing (GCM)



- Discretization mesh (q_1, q_2): 40 fm^2
- Several 1qp states at each deformation.

- Total number of one-quasiparticle states used:
  - positive parity: 100 states.
  - negative parity: 60 states.

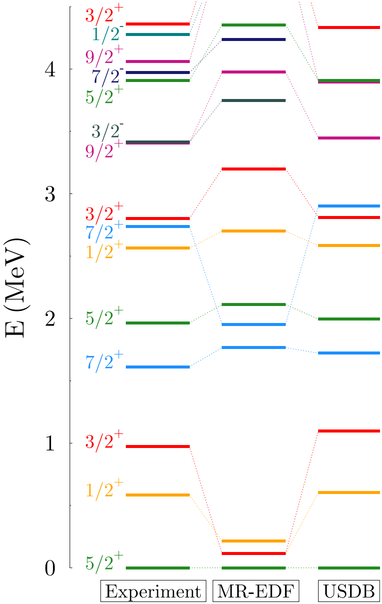
Ground-state properties

	J^π	Binding energy (MeV)	Q_s ($e\,\mathrm{fm}^2$)	μ (μ_N)
Experiment	$\frac{5}{2}^+$	-205.587	20.1(3)	$-0.85545(8)$
MR-EDF	$\frac{5}{2}^+$	-221.875	23.25	-1.054

- No effective charge or effective g-factor!

- Experiment: Nuclear Data Sheets **110** 1691 (2009)

Low-energy spectrum



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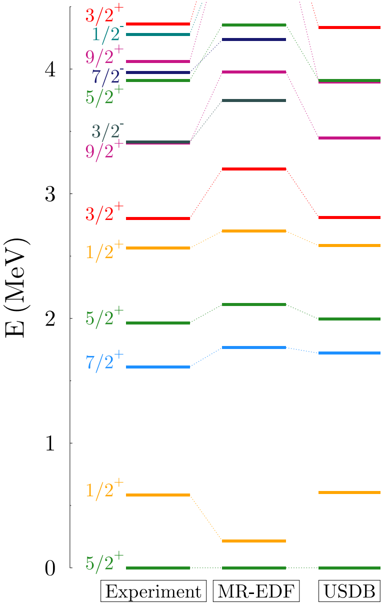

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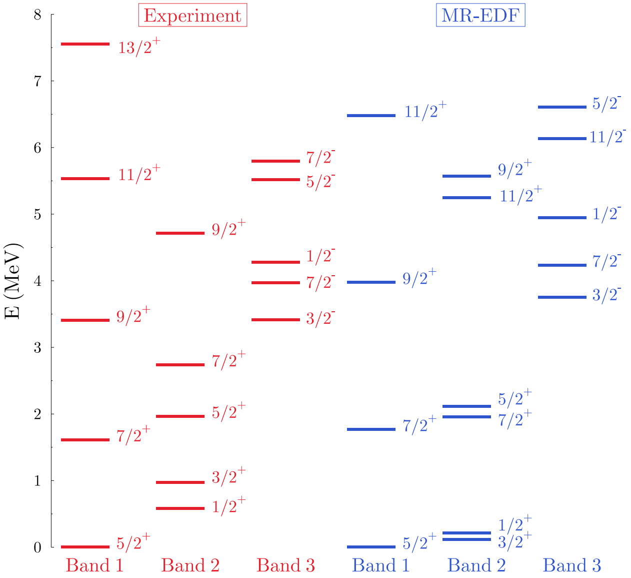
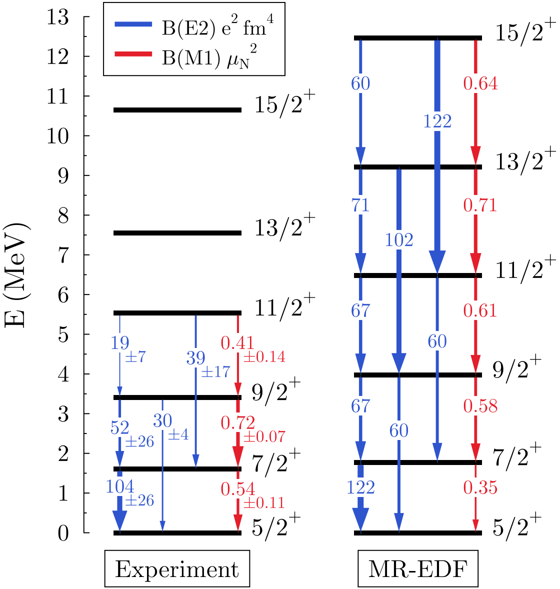
Rotational bands



Ground-state band



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Conclusion

Calculation of ^{25}Mg:

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Goals of the PhD:

- ✔ Treatment of even-even and odd-even (and even odd-odd) nuclei on the same footing.
- ✔ MR-EDF calculations with a Hamiltonian-based functional.
- ✔ Spectroscopy of odd-mass nuclei.
- ✘ World domination.

Outlook

- Urgent need for a better Skyrme parametrization.
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- And a lot of other stuff as well . . .