Multi-Reference Calculations for Odd-Mass Nuclei

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DE LA RECHERCHE À L'INDUSTRIE
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DSM - DAM

Table of contents

Table of contents

We define an EDF (≡ effective Hamiltonian).

↓

We create a set of one-quasiparticle states:
$\{|\Phi_a\rangle,\ a = \ldots\}$

↓

We project each of them on the good quantum numbers:
$\{|JMNZP\epsilon, a\rangle,\ a, J, P, \epsilon = \ldots\}$.

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We diagonalize the (effective) Hamiltonian between the projected states: $\{|JMNZP\xi\rangle,\ J, P, \xi = \ldots\}$.

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Energy functional

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

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

- $|\Phi_a\rangle$, $|\Phi_b\rangle$: 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

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

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

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

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Symmetries of quasiparticle states

- Number parity: $\hat{\Pi}_A|\Phi_a\rangle = \pi_a|\Phi_a\rangle$ $\quad (\hat{\Pi}_A = e^{-i\pi\hat{A}})$

Subgroup of D_{2h}^{TD} :

- Signature: $\hat{R}_x|\Phi_a\rangle = \eta_a|\Phi_a\rangle$ $\quad (\hat{R}_x = e^{-i\pi\hat{J}_x})$
- Parity: $\hat{P}|\Phi_a\rangle = p_a|\Phi_a\rangle$
- y-Time Simplex: $\hat{S}_y^T|\Phi_a\rangle = |\Phi_a\rangle$ $\quad (\hat{S}_y^T = \hat{R}_y\hat{P}\hat{T})$

- odd A: $\pi_a = -1$, $\eta_a = \pm i$, $p_a = \pm 1$

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: $\langle\Phi_a|\hat{Q}|\Phi_a\rangle = Q$

- Self-consistent problem: solved by an iterative procedure.
- Solved for different values of Q and/or $\hat{\beta}^\dagger_a$

Outline of the EDF method

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Symmetry restoration

Conservation of the neutron and proton numbers:

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

$\Rightarrow$ Projection on neutron and proton numbers.

Conservation of total angular momentum:

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

$\Rightarrow$ Projection on total angular momentum.

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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.

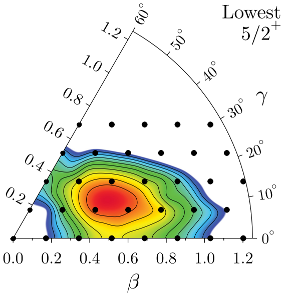
$$\frac{\delta}{\delta F_\xi^{\Lambda *}(i,\epsilon)} \left(\frac{\langle \Lambda M \xi | \hat{H} | \Lambda M \xi \rangle}{\langle \Lambda M \xi | \Lambda M \xi \rangle} \right) = 0 \Longrightarrow F_\xi^\Lambda(i,\epsilon) \text{ et } E_\xi^\Lambda(\Omega_I)$$

Table of contents

Motivations

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

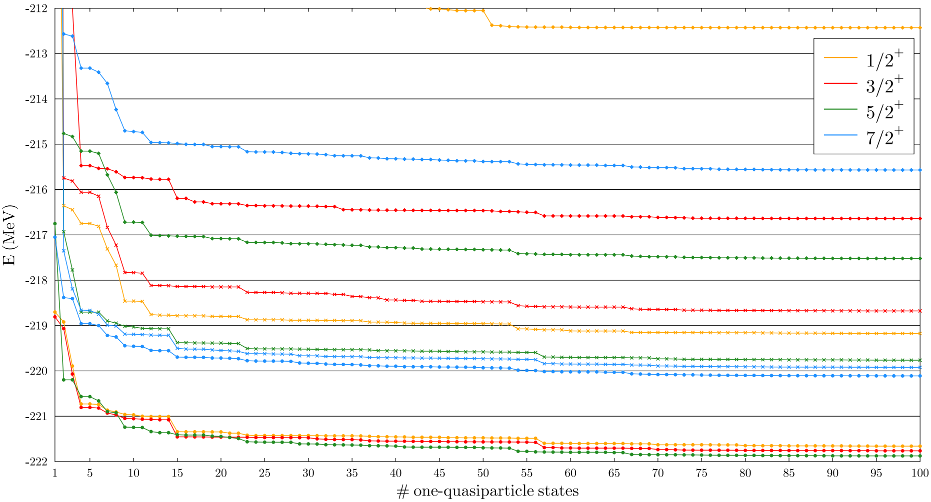
Characteristics of the Configuration Mixing (GCM)



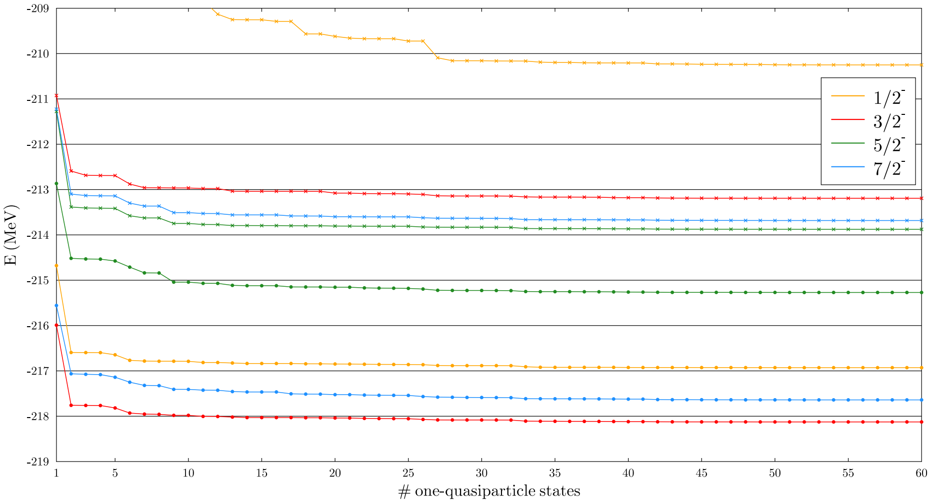
- Discretization mesh (q_1, q_2): 40 fm^2
- Several 1qp states at each deformation.

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

Convergence analysis



Convergence analysis II



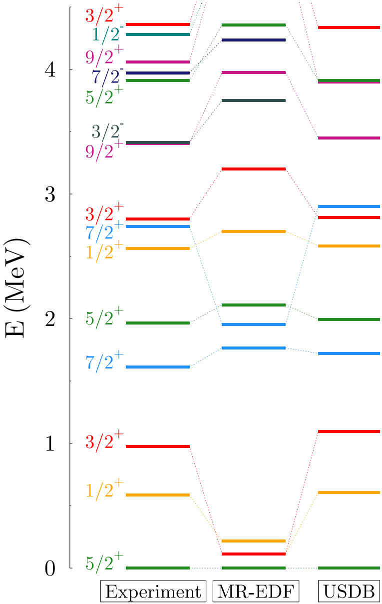
Ground-state properties

	J^π	Binding energy (MeV)	Q_s ($e\,\text{fm}^2$)	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



- Shell Model: USDB with NushellX.
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- Not as good as Shell Model but less parameters!
  And not fitted specifically to the sd shell!
- Negative parity states!

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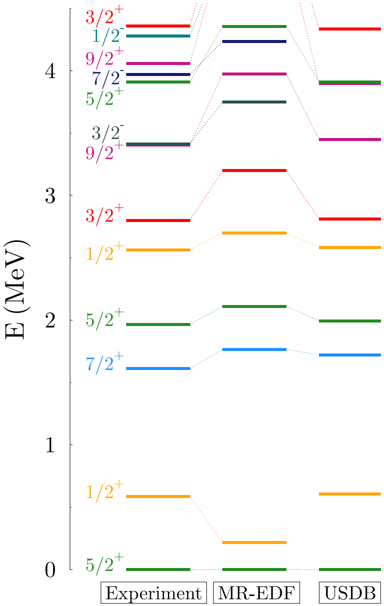

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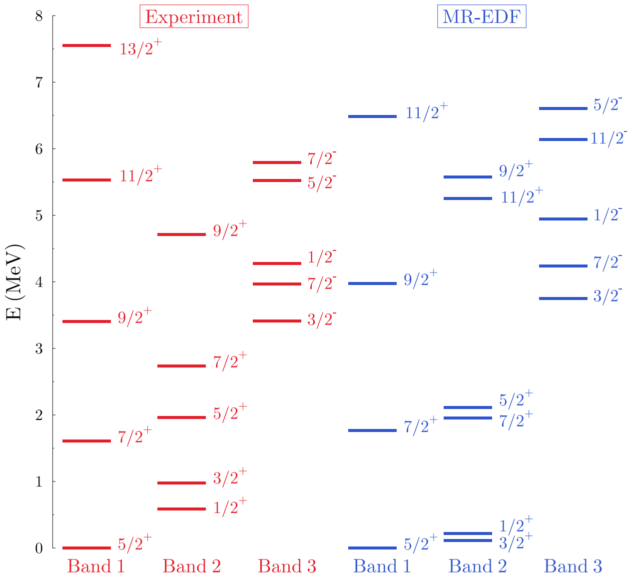
Rotational bands



Ground-state band

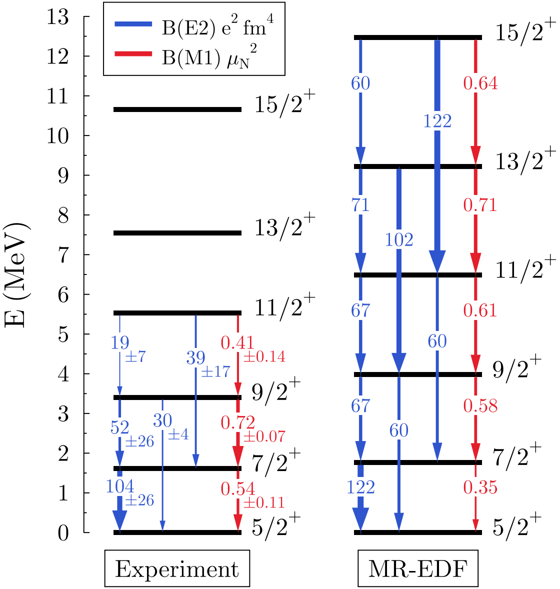


Table of contents

Conclusion

Calculation of ^{25}Mg:

- Overall reasonable description ...
- ... especially considering the limited quality of SLyMR0.
- Proof of principle of the method.

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Goals:

- ✔ 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.

Outlook

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  → **underway**: Skyrme with gradient three-body terms.

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- More calculations and heavier nuclei.
  → speedup of the programs.