Configuration mixing of symmetry-restored odd-quasiparticle excitations for the description of odd-mass nuclei

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ESNT - March 2nd 2017

DE LA RECHERCHE À L'INDUSTRIE

cea

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Espace de Structure Nucléaire Théorique
DSM - DAM

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Introduction

- Aim: description of the low-energy structure of odd-mass nuclei

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  - ◇ Configuration mixing → in the spirit of GCM
  - ◇ Symmetry restoration → projection technique

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  . . . but present generation of functionals is too limited

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- Closely related to the talks given by J.L. Egido and M. Bender

Degrees of freedom

- Degrees of freedom treated
  - Pairing
  - Triaxial deformations
  - One-quasiparticle excitations

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  - Pairing
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- Next degrees of freedom to be included?
  - Cranking (possible with the actual code)
  - Octupole deformation
  - Three-quasiparticle excitations (possible with the actual code)

MR EDF "Algorithm"

We define an EDF (≡ effective Hamiltonian)

↓

We create a set of states $\Omega \equiv \left\{ |\Phi_i\rangle, i = \dots \right\}$

↓

We project each of them on the good quantum numbers $\left\{ |\Psi^{JMNZ}_{\epsilon i}\rangle, J\epsilon, i \right\}$

↓

We diagonalize the (effective) Hamiltonian between the projected states $\left\{ |\Theta^{JMNZ}_{\xi\Omega}\rangle, JMNZ, \xi \right\}$

↓

We calculate observables

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Energy functional

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

$$\rho^{ab} = \frac{\langle \Phi_a | c^\dagger c | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle} \qquad \kappa^{ab} = \frac{\langle \Phi_a | c c | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle} \qquad \kappa^{ba\,*} = \frac{\langle \Phi_a | c^\dagger c^\dagger | \Phi_b \rangle}{\langle \Phi_a | \Phi_b \rangle}$$

- $|\Phi_i\rangle$ Bogoliubov quasiparticle state $\begin{pmatrix} \beta_i \\ \beta_i^\dagger \end{pmatrix} = \begin{pmatrix} U_i^\dagger & V_i^\dagger \\ V_i^T & U_i^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$

- $\mathcal{E}_{\text{nuc}}$ **directly and uniquely** determined by H
  $\Rightarrow$ no density-dependent interaction

Nuclear effective hamiltonian

$$H = K + V_{\text{Coul}} + V_{\text{Sky}}$$

- K: kinetic energy (+ center of mass corr.)
- V_{Coul}: Coulomb interaction
  All terms taken into account **exactly**
  Computationally most time-consuming part of the calculation
- V_{Sky}: Skyrme pseudopotential - **Highly schematic**

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SLyMR0 and SLyMR1 parametrizations

Sadoudi *et al.* Physica Scripta T154 014013 (2013)
Sadoudi *et al.* Phys. Rev. C 88, 064326 (2013)
R. Jodon, PhD thesis, Université Lyon 1 (2014)

Symmetries of quasiparticle states

- Calculations on 3d Lagrange mesh in Cartesian coordinates

  D. Baye and P.-H. Heenen, J.Phys.A:Math.Gen. 2041 (1986)

- Impose symmetries of a subgroup of D_{2h}^{TD}

  x-signature
  parity
  y-time simplex

  } Triaxial deformations and cranking

Minimization of quasiparticle states

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

Constraints

- Neutron number $\langle\Phi_a|N|\Phi_a\rangle = N_0$
- Proton number $\langle\Phi_a|Z|\Phi_a\rangle = Z_0$
- Quadrupole deformation $\langle\Phi_a|Q|\Phi_a\rangle = Q_0$
- Blocking structure $|\Phi_a\rangle = \beta_1^\dagger \dots \beta_n^\dagger|\tilde{0}\rangle$

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Solved for different values of Q_0 & $\beta_1^\dagger \dots \beta_n^\dagger$

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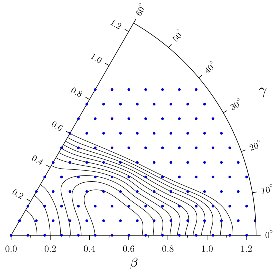
First odd-mass calculation: $^{25}_{12}\mathrm{Mg}$

- Interests
  - Proof of principle
  - Light nucleus (*sd* shell) with a simple structure
  - Bally *et al.* PhysRevLett 113, 162501 (2014)

- Theoretical calculations with
  - SLyMR0 parametrization
  - LN to enforce pairing
  - Triaxially deformed one-quasiparticle states
  - Projection on J, N, Z + triaxial & 1qp configuration mixing

Strategy at the single-reference level

- Select a discretization of triaxial deformations (β, γ)



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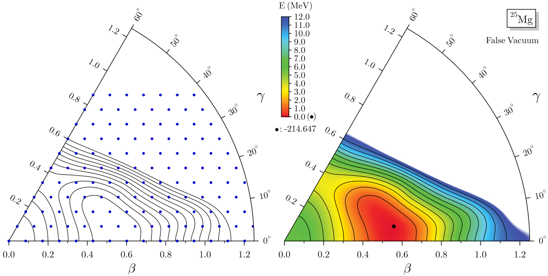

- Calculate "false vacuum" at each deformation

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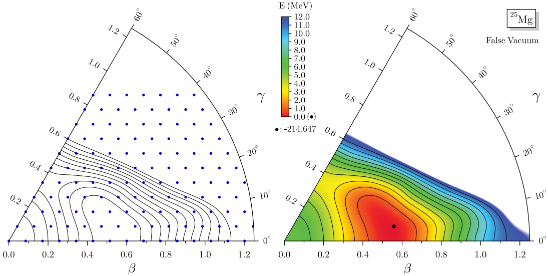
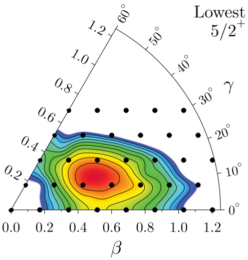


- Calculate "false vacuum" at each deformation

- Block self-consistently many one-quasiparticle states ...
  ... those which appeared to be of lowest energy
  - $\approx$ 600 positive parity states
  - $\approx$ 200 negative parity states

How to select the states to include in the mixing?



- Pick a sparser discretization of triaxial deformations

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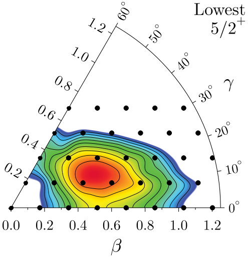
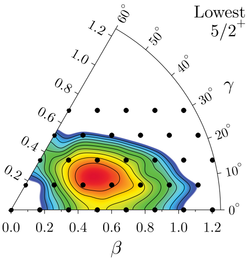


- Pick a sparser discretization of triaxial deformations
- At least the lowest one at each deformation

How to select the states to include in the mixing?



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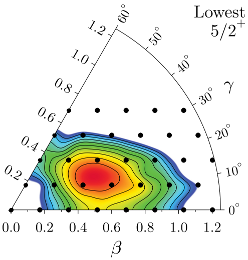

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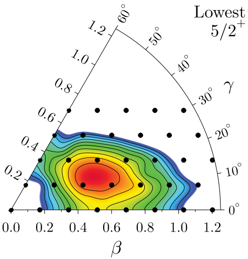


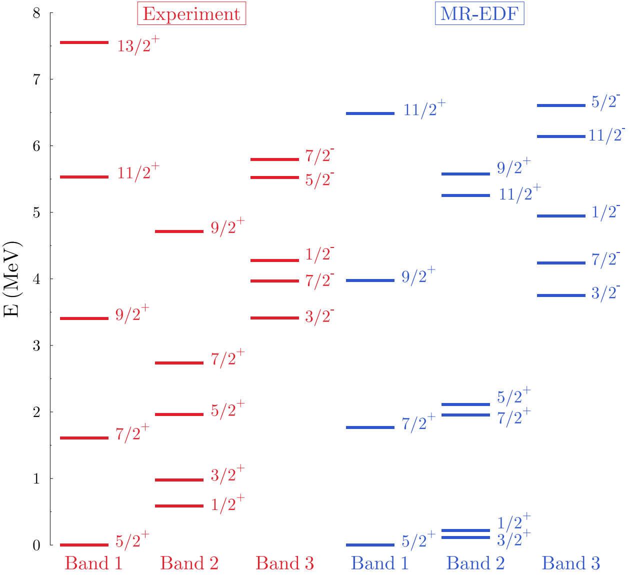
- Pick a sparser discretization of triaxial deformations
- At least the lowest one at each deformation
- Then from energy & structure of projected states
- How many CPU hours do I have?
- Total number of states selected
  - 100 positive parity states
  - 60 negative parity states

Ground-state properties

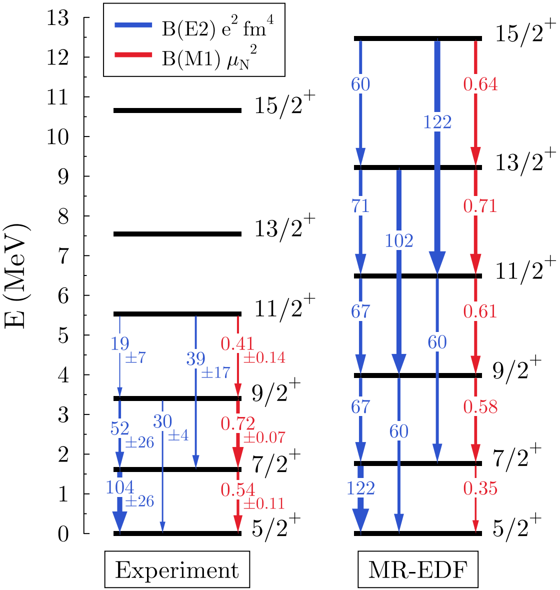
	J^π	Binding energy (MeV)	Q_s ($e\,\text{fm}^2$)	μ (μ_N)
Experiment	$\frac{5}{2}^+$	−205.587	20.1(3)	−0.85545(8)
MR EDF	$\frac{5}{2}^+$	−221.875	23.25	−1.054

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

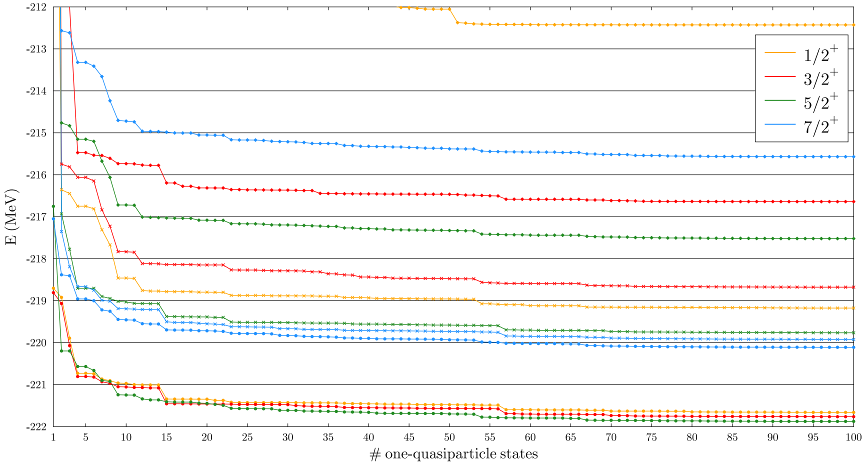
Rotational bands



Ground-state band

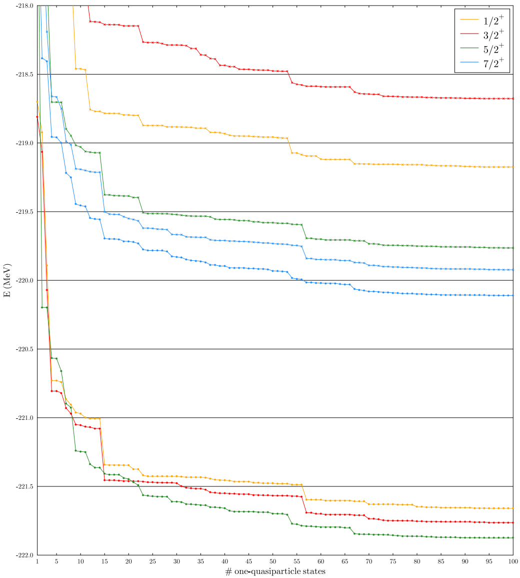


Convergence of lowest positive parity states



- States added by increasing order of non-projected energy

Convergence of lowest positive parity states



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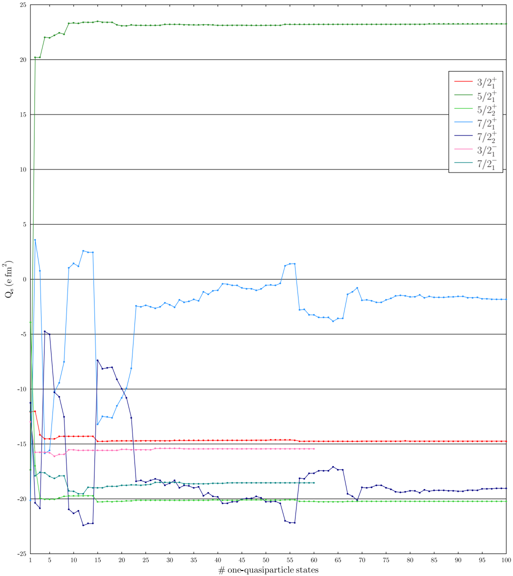

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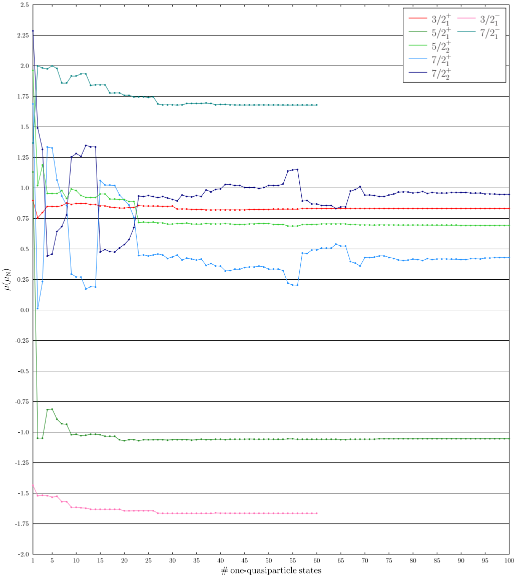

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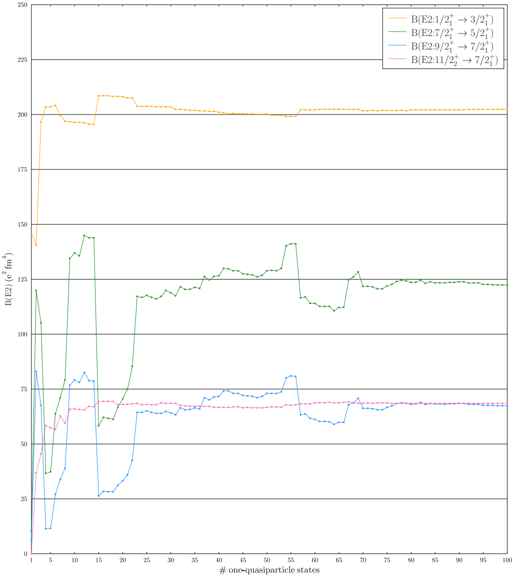
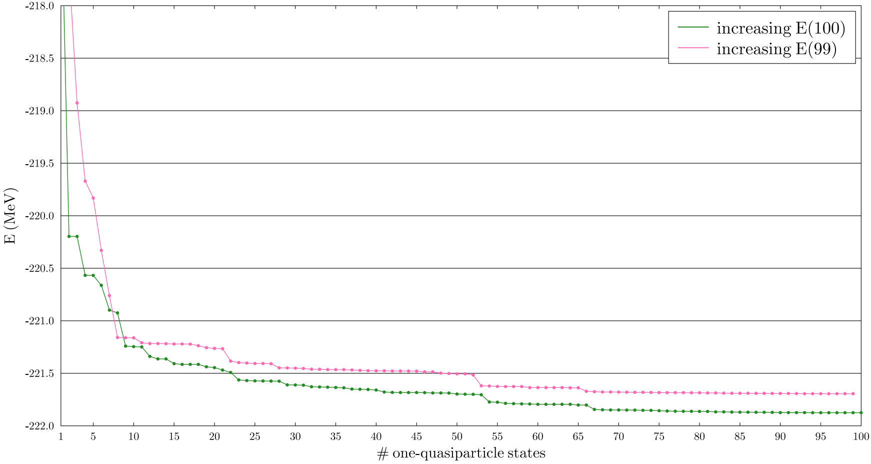
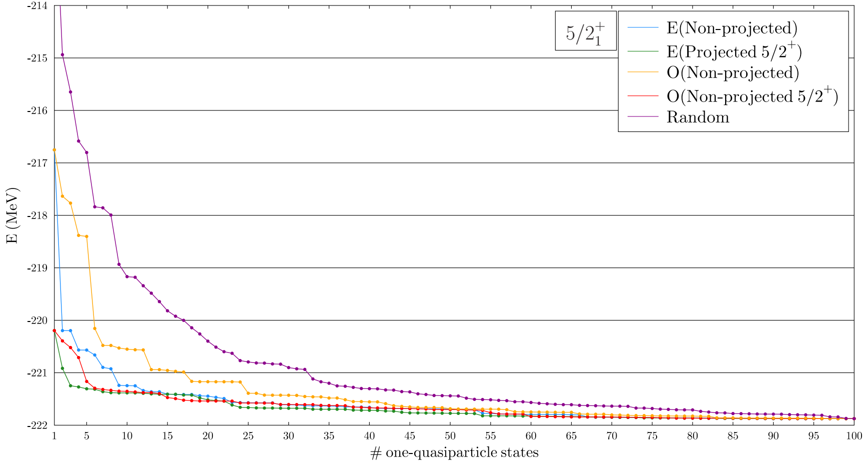


Some states are more important than others



How to determine the most important states?



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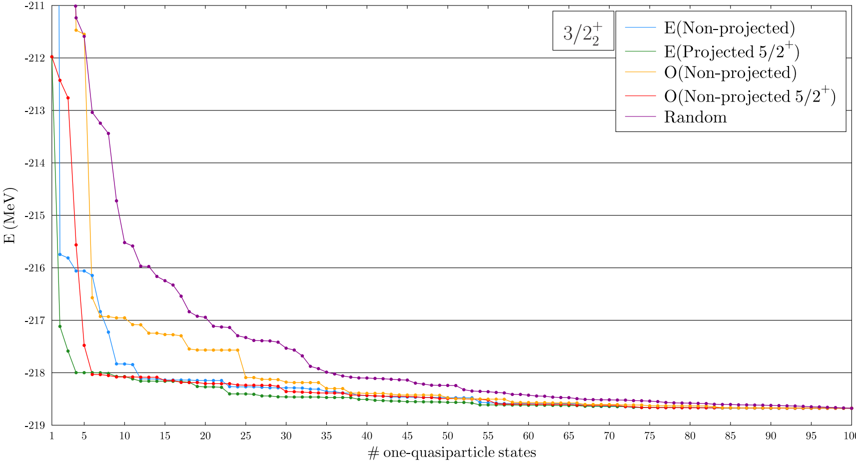

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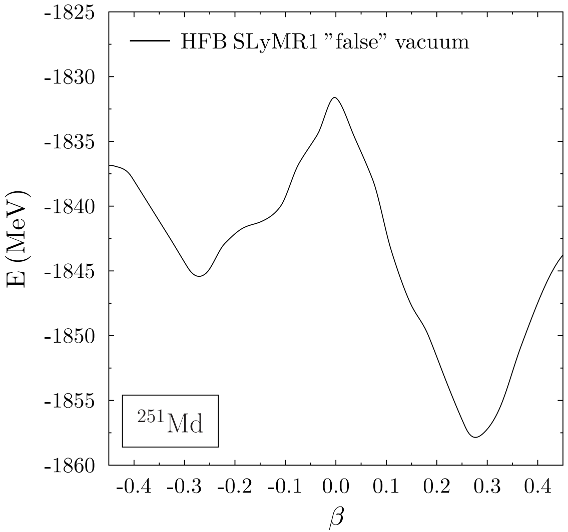
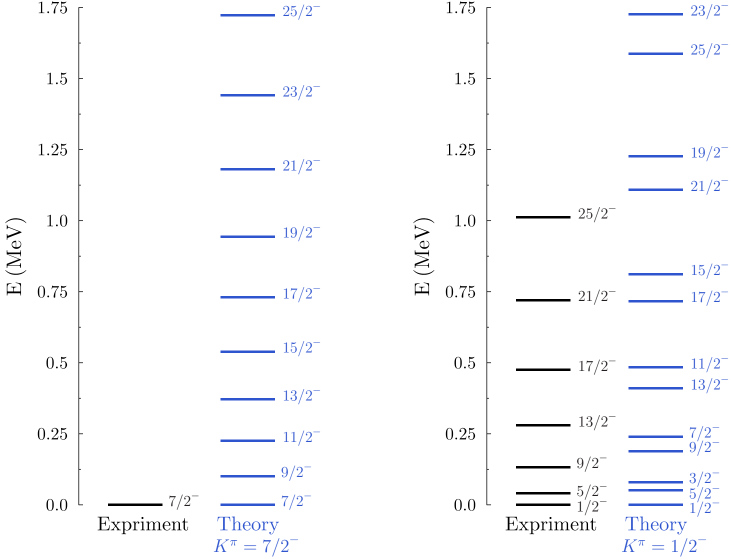
Going heavy with $^{251}_{101}\mathrm{Md}$

- (MR) EDF only microscopic method for heavy and superheavy nuclei
- Experimental progress in spectroscopy of transactinides
  → soon S^3 at GANIL
- Theoretical calculations with
  - SLyMR1 (include three-body gradients)
  - Projection on J, N, Z of one-qps with axial deformations
  - No GCM yet as just a test of the interaction & code
    P.-H. Heenen *et al.* EPJ Web of Conferences 131, 02001 (2016)



HFB SLyMR1 "false" vacuum
^{251}Md
E (MeV)
-1825
-1830
-1835
-1840
-1845
-1850
-1855
-1860
-0.4
-0.3
-0.2
-0.1
0.0
0.1
0.2
0.3
0.4
β

Going heavy with $^{251}_{101}\mathrm{Md}$



- Experiment: A. Chatillon *et al.* Phys. Rev. Lett. 98, 132503 (2007)

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Impressions and interrogations

- Calculations of odd nuclei are possible ... but painful

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- Not yet sure of the best strategy for qp excitations
  - All self-consistent or adiabatic + perturbative on top?
  - How to determine most important qp exictations?
  - How many needed?

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  - ◇ All self-consistent or adiabatic + perturbative on top?
  - ◇ How to determine most important qp exictations?
  - ◇ How many needed?
- Need to improve moments of inertia → cranking?
- Projection & GCM cannot overcome large deficiencies of EDF → single-particle spectrum

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