MICROSCOPIC CALCULATIONS OF FISSION BARRIERS IN THE ACTINIDE REGION

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# INTRODUCTION

#### AIM OF RESEARCH

- calculation of fission barrier heights of odd-mass nuclei in the actinide region
- dependence of the inner barrier height on the K<sup>π</sup> quantum numbers (assuming K is conserved along fission process)
- study of the energy spectra in the ground-state and fission-isomeric wells and transition (discrete) states at the top of the first barrier





#### HARTREE-FOCK (HF) PLUS PAIRING (BCS)

- breaking of time-reversal symmetry (due to the addition of one unpaired nucleon)
  - proper account of the effect through self-consistent blocking (SCB) calculations
  - vs. the Equal Filling Approximation (EFA); see e.g.
    - F. de la Iglesia, V. Martin, S. Perez Martin and L. M. Robledo, AIP Conf. Proc. 1175, 199 (2009) : <sup>239</sup>Pu
    - S. Perez Martin and L. M. Robledo, Int. J. Mod. Phys. E 18 788-797 (2009): <sup>235</sup>U
    - Koh Meng Hock, L. Bonneau and P. Quentin, EPJ Web of Conferences 62, 04004 (2013)
- blocking of a single-particle state with specific K<sup>π</sup> quantum numbers, and taking the lowest-energy solution





#### DEFINING A PAIR STATE IN BCS SCHEME

• Definition of a "Kramers quasi-pair" ( $|i\rangle$ ,  $|\tilde{i}\rangle$ ):

$$\begin{split} \hat{h}_{\rm HF}|i\rangle &= \boldsymbol{e}_i|i\rangle \qquad \hat{J}_z|i\rangle = \Omega_i|i\rangle \quad \text{with } \Omega_i > 0 \\ \hat{h}_{\rm HF}|\tilde{i}\rangle &= \boldsymbol{e}_i|\tilde{i}\rangle \qquad \hat{J}_z|\tilde{i}\rangle = \Omega_{\tilde{i}}|\tilde{i}\rangle \quad \text{with } \Omega_{\tilde{i}} = -\Omega_i < 0 \\ \left|\langle \bar{i}|\tilde{i}\rangle\right| \text{ maximum (close to 1 in practice)} \end{split}$$

• Energy splitting in a Kramers quasi-pair:  $\delta e_i = e_i - e_{\tilde{i}}$ 



#### NUMERICAL PARAMETERS

- effective nucleon-nucleon interaction : Skyrme SkM\* force
- the single-particle states are expanded on a cylindrical harmonic-oscillator basis with a basis size,  $N_0 = 14$
- seniority force with pairing strength in the BCS scheme where the pairing strengths were fitted to the odd-even binding energy differences of some actinide nuclei, with retained values of  $G_0$ (neutron) =  $G_0$ (proton) = -16.0 MeV
  - pairing window up to  $\epsilon_F$  + 6.0 MeV with a diffuseness parameter of 0.2 MeV





#### UNIFIED MODEL PICTURE

- HFBCS solution  $|\Psi_K\rangle$  as intrinsic state
- rotational correction to intrinsic energy
- Coriolis coupling for  $K = \frac{1}{2}$  states
- energy of the  $J^{\pi}$  member of the  $K^{\pi}$  rotational band:

$$E_J = E_{K=J} + \frac{\hbar^2}{2\mathcal{I}} \Big[ J(J+1) - K(K+1) \Big]$$

with

$$E_{J=K} = \underbrace{\langle \Psi_{K} | \hat{H} | \Psi_{K} \rangle}_{\text{intrinsic energy}} - \underbrace{\frac{\hbar^{2}}{2\mathcal{I}} \Big( \langle \Psi_{K} | \hat{\mathbf{J}}^{2} | \Psi_{K} \rangle - K(K+1) \Big)}_{\text{rotational correction}} - \underbrace{\frac{\hbar^{2}}{2\mathcal{I}} \delta_{K\frac{1}{2}}(-)^{J+\frac{1}{2}} (J+\frac{1}{2}) a}_{\text{Coriolis coupling}}$$

 $\mathcal{I}$  is the moment of inertia calculated for the even-even core (preliminary)





#### ONE-QUASIPARTICLE BANDHEADS IN <sup>235</sup>U (GS WELL)







### ONE-QUASIPARTICLE BANDHEADS IN <sup>239</sup>PU GS WELL







### ONE-QUASIPARTICLE BANDHEADS IN <sup>239</sup>PU SD WELL







#### ROTATIONAL BANDS AT <sup>239</sup>PU FIRST SADDLE







#### FISSION BARRIERS FOR FIXED $K^{\pi}$

Relative energies of first saddle point and second (SD) minimum with respect to GS minimum for various  $K^{\pi}$ :

<sup>235</sup> U			<sup>239</sup> Pu		
K <sup>π</sup>	EA	E <sub>SD</sub>	EA	E <sub>SD</sub>	· Deformation energy surface
1/2+	6.6	2.6	7.4	1.7	
7/2-	6.8	2.5	7.9	2.5	
5/2 <sup>+</sup>	5.8	1.4	7.0	0.9	E <sub>sD</sub>
7/2+	_	_	5.9	1.6	





#### **EFFECT OF TIME-REVERSAL SYMMETRY BREAKING**

Difference between first-fission-barrier heights without (EFA) and with (SCB) time-reversal symmetry breaking in the selfconsistent blocked HFBCS solution for various  $K^{\pi}$ :

$\mathbf{K}^{\pi}$	$E_A(SCB) - E_A(EFA)$ (keV)
1/2+	20
7/2-	20
5/2+	0





# CONCLUSIONS

 The calculated spectra compare favorably with experimental data in GS and SD wells
⇒ reasonable class-I, class-II and transition states of rotational character







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  ⇒ reasonable class-I, class-II and transition states of rotational character
- **②** The inner barrier height can vary significantly with  $K^{\pi}$
- EFA seems justified for calculations of fission-barrier heights (not for spectroscopic properties like magnetic moments)







### PERSPECTIVES

- Extend study to second saddle point (outer fission barrier)
- Improve moment of inertia for the core:
  - core polarization
  - pairing quenching because of unpaired nucleon (blocking)
- Restore particle-number symmetry broken by BCS
   ⇒ Highly Truncated Diagonalization Approach (HTDA)
   ≈ highly truncated shell model based on a mean-field
   solution
- Account for vibrational degrees of freedom, for example in the HTDA approach

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• Extension to odd-odd compound nuclei





Fission-isomeric (SD) well of 235U





