3rd rencontre PhyNuBE

# Structure and angular momentum at scission from microscopic models

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#### Hartree-Fock

$$\hat{h}_{MF}(\rho) |\varphi_i\rangle = \epsilon_i |\varphi_i\rangle$$

with  $\hat{h}_{MF}(\rho)$  the self-consistent mean-field Hamiltonian



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$$i\hbar \frac{d}{dt} |\varphi_i\rangle = (\hat{h}_{MF}(\rho) - \epsilon_i) |\varphi_i\rangle$$

#### Application of mean-field dynamics



Reactions



#### Fission





#### Fission



#### Application of mean-field dynamics





#### Fission



#### Uncertainty principle

$$\Delta X_{c.m.} \Delta P_{c.m.} \geq \hbar/2$$

# Uncertainty principle

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**TDHF** evolution

Exact evolution



### Uncertainty principle

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#### Limitation of the TDHF evolution

Classical description of the collective variable



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Classical description of the collective variable

### Limitation

- no tunneling
- no fluctuation of the collective observable



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#### Limitation of the TDHF evolution

Classical description of the collective variable

#### Limitation

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#### Important

The same is true with pairing (TDHF+BCS, TDHFB)

#### Time-dependent density functional theory - TDDFT

#### TDHF

- Independent particle
- Initialisation :  $\hat{h}_{MF} |\phi_i\rangle = \epsilon_i |\phi_i\rangle$
- Evolution :  $i\hbar \frac{d\rho}{dt} = [h_{MF}, \rho]$

#### TDHFB - TDSLDA

- Pairing correlation
- Quasi-particles :  $|\omega_{\alpha}\rangle = \begin{pmatrix} U_{\alpha} \\ V_{\alpha} \end{pmatrix}$
- One-body  $\rho$  and simplified two body density  $\kappa$

• Evolution :  
$$i\hbar \frac{d|\omega_{\alpha}\rangle}{dt} = \begin{pmatrix} h & \Delta \\ -\Delta^* & -h^* \end{pmatrix} |\omega_{\alpha}\rangle$$

Self consistent theory - Effective Skyrme functional





G. Scamps, C. Simenel, D. Lacroix, PRC 92, 011602(R) (2015).



TDHF

G. Scamps, C. Simenel, D. Lacroix, PRC 92, 011602(R) (2015).



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#### Impact of pairing

Pairing is a lubricant for fission

J. Phys. G: Nucl. Part. Phys. 47 (2020) 113002









#### Empirical behaviour of actinide nuclei





J.P. Unik, J.E. Gindler, J.E. Glendenin et al. : Proc. Phys. and Chem. of Fission IAEA Vienna, Vol II, 20 (1974)



#### Empirical behavior of actinide nuclei





#### Motivation

How can we understand this behaviour? Interplay between structure and reactions?



#### Second : TDHF+BCS





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#### Comparison with experimental data





#### Conclusion :

The TDHF+BCS calculation reproduces well the Z=54 behavior. But why?



# <sup>240</sup>Pu



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Similar effect on fusion reaction :



C. Simenel, M. Dasgupta, D. J. Hinde, and E. Williams, Phys. Rev. C 88, 064604 (2013).

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S. Ebata, and T. Nakatsukasa, Phys. Scr. 92 (2017)



#### Results from systematic calculation

In both calculations, the region Z  $\simeq$  56, N  $\simeq$  88 is favorable for octupole deformation.

#### **Experimental results**

<sup>144</sup>Ba is found to be octupole in its ground state. Burcher et al. PRL 116 (2016).


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# Single particle energy



# Single particle energies



# **Experimental results**



# Conclusion



# Mechanism

- The Nucleus-Nucleus interaction at the scission configuration favors the octupole shapes
- $\bullet\,$  Shell structure favors octupole shape in the region Z  $\simeq$  52-56, N  $\simeq$  84-88
- $\bullet\,$  Actinide fission fragments are driven in the region Z  $\simeq$  54, N  $\simeq 86$

G. Scamps, C. Simenel, Nature 564, 382 (2018).





G. Scamps C. Simenel, PRC 100, 041602(R) (2019)



Schmidt, PLB 825, 136859 (2022)

# Scission point model





Spin of the Fragments



# J. N. Wilson, Nature, 590, 566 (2021)

- The average spin follows a sawtooth shape
- No correlations between the spins of the fragments

## Spins are mostly perpendicular to the fission axis



FIG. 9. The points are the calculated populations of the various *m* substates of the 2<sup>1</sup> level in <sup>14</sup> Hig. These values were determined using the fitted experimental angular distribution of the 2<sup>n</sup>  $-0^{\circ}$   $\gamma$  ray. The solid line represents the predicted population of the m states as calculated from the statistical-model analysis of the deexcitation process using Eqs. (4) and (5) with an assumed value of B = 6 [Eq. (3)] for the initial angular momentum distribution.

J. B. Wilhelmy, E. Cheifetz, R. C. Jared, S. G. Thompson, H. R. Bowman, and J. O. Rasmussen Phys. Rev. C 5, 2041 (1972)

- Thermal excitations
- Quantum fluctuations
- Coulomb force
- Breaking of the neck

# **Tilting Mode**



Illustration from B. John, J. Phys., 85, 2, (2015).

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# Tilting Mode



Illustration from B. John, J. Phys., 85, 2, (2015).

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# **Twisting Mode**



Illustration from B. John, J. Phys., 85, 2, (2015).

- Thermal excitations
- Quantum fluctuations
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- Breaking of the neck

# Wriggling Mode



Illustration from B. John, J. Phys., 85, 2, (2015).

- Thermal excitations
- Quantum fluctuations
- Coulomb force
- Breaking of the neck

# Bending Mode



Illustration from B. John, J. Phys., 85, 2, (2015).



S. Franke-Arnold, et al. New Journal of Physics 6, 103 (2004)





# Projection method

$$\begin{aligned} |a_{J}^{F}|^{2} = & \frac{2J+1}{2} \int_{0}^{2\pi} \sin(\beta) \\ P_{J}(\cos(\beta)) \langle \Psi | e^{\frac{-iJ_{x}^{F}\beta}{\hbar}} | \Psi \rangle \end{aligned}$$

 $\beta_{2}^{f} = 0.1$ 

 $\beta_{1}^{\xi} = 0.5$ 



G. F. Bertsch, T. Kawano, and L. M. Robledo, PRC 99, 034603 (2019)

# Problem of interpretation

- The spin cut-off distribution is already present in the ground state of even-even deformed nuclei if symmetry are not restored
- $\hat{J}^2$  and  $\hat{P}(J)$  are 2 and N-body operators
- Fragments do not rotate in dynamical approaches



A. Bulgac, et al. PRL 116, 122504 (2016)

# Problem of interpretation

- The spin cut-off distribution is already present in the ground state of even-even deformed nuclei if symmetry are not restored
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# Potential as a function of the light fragment angle



The azimuthal angle doesn't have an important role.

# Method

- One body-evolution One body-observable
- Breaking of the axial symmetry at scission

#### Results

- Agreement between the dynamic and the FHF potential
- Repulsive Coulomb torque; attractive NN torque
- Small effect of the azimuthal angle

# Limitation

- Classical evolution
- No prescription for the initial angle
- Frozen Hartree-Fock approximation for the initial pre-fragment

# Frozen Hartree-Fock potential



Two torques :

- attractive nucleus-nucleus torque
- repulsive Coulomb torque



#### Hamiltonian

$$\hat{H}(D) = \frac{\hbar^2}{2I_H}\hat{L}_H^2 + \frac{\hbar^2}{2I_L}\hat{L}_L^2 + \frac{\hbar^2}{2I_{\Lambda}(D)}\hat{\Lambda}^2 + \hat{V}(\hat{\Theta}_H, \hat{\Theta}_L, \hat{\varphi}, D)$$
  
Solved in basis  $|L_H, m, L_L, -m\rangle$ 

G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616(2023).

Similar to the orientation pumping mechanism model Mikhailov, I. N., and Quentin, P. (1999). On the spin of fission fragments, an orientation pumping mechanism. Physics Letters B, 462(1-2), 7-13.



#### Effect of quadrupole deformation >> effect of $Z_1Z_2$

TABLE II. Average spin $(L^2)^{\frac{1}{2}}$  in unit of  $\hbar$  for the three fission fragments at scission (D = 21 fm) and at large distances. The last two columns show the same quantity with an MOI divided by 2.

Nucleus	Scission	Final	Scission $(I_{\frac{1}{2}})$	Final $(I_{\frac{1}{2}})$
<sup>108</sup> Ru	9.28	12.31	7.24	10.38
<sup>144</sup> Ba	10.04	10.95	7.70	8.66
<sup>96</sup> Sr	7.74	9.30	6.03	7.62

also J. Randrup, PRC 108, 064606 (2023) : increase of 1 to 3  $\hbar$  due to the Coulomb torque.



- <sup>132</sup>Sn is found in ground-state
- The collective Hamiltonian model with  $\beta_2=0.42$  reproduces the experimental  $\gamma$ -spectrum



A. Francheteau, L. Gaudefroy, G. Scamps, O. Roig, V. Méot, A. Ebran, and G. Bélier, PRL 132, 142501 (2024).

#### Correlation between the angular momentum



# <sup>144</sup>Ba+<sup>96</sup>Sr

- No or small correlation observed in the magnitude of the angular momentum.
- More angular momentum for the heavy fragment



# Discussion



- Pear-shaped deformation plays an important role at scission. G. Scamps C. Simenel, Nature 564, pages 382–385 (2018)
- Octupole deformation makes the angular potential stiffer which increase the zero-point motion → more angular momentum

G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).



#### TDDFT (in 2022) vs Freya



A. Bulgac, I. Abdurrahman, K. Godbey, and I. Stetcu, Phys. Rev. Lett. 128, 022501(2022).



G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).

### Geometry

- Small azimuthal correlation
- Spin are perpendicular to the fission axis
- Complex pattern in the opening angle, different from previous model
- Slightly more wriggling mode than bending because wriggling potential is more rigid

## Method

- $\bullet~$  Quantal collective model  $\rightarrow$  beyond one-body
- Time-dependent evolution of a wave-packet
- Microscopic potential with FHF

#### Results

- No strong correlation of the magnitude and direction of the spins
- Both spins are oriented in the plane perpendicular to the fission axis.
- $\bullet\,$  The Coulomb interaction induces an increase of the angular momentum by 1 to 3  $\hbar\,$
- The octupole deformation increases the angular momentum generated at scission

# Limitation

- Frozen approximation
- Initial conditions

G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).

# Projection method

Projection on the spin and K number (Projection of the spin on the fission axis)

$$\begin{split} \hat{P}_{MK}^{S} &= \frac{(2S+1)}{16\pi^2} \int \! d\Omega \mathcal{D}_{MK}^{S*}(\Omega) \, e^{i\alpha \hat{S}_z} e^{i\beta \hat{S}_y} e^{i\gamma \hat{S}_z}, \\ P(S_F, K_F) &= \langle \Psi | \hat{P}_{K_F K_F}^{S_F} | \Psi \rangle, \end{split}$$

Calculation of the overlap : G. F. Bertsch and L. M. Robledo, PRL 108, 042505 (2012)

$$\langle \Psi | \hat{R} | \Psi \rangle = \frac{(-1)^n}{\prod_{\alpha}^n v_{\alpha}^2} \mathrm{pf} \begin{bmatrix} V^T U & V^T R^T V^* \\ -V^{\dagger} R V & U^{\dagger} V^* \end{bmatrix}$$

Optimized Pfaffian calculation : M. Wimmer, ACM Trans. Math Softw. 38, 30 (2012).


G.scamps, I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, PRC 108 (6), L061602



G.scamps, I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, PRC 108 (6), L061602.

$$arphi_{HL} = \arccos\left(rac{\Lambda(\Lambda+1) - S_H(S_H+1) - S_L(S_L+1)}{2\sqrt{S_H(S_H+1)S_L(S_L+1)}}
ight)$$

$$P(\Lambda, S_H, S_L) = \sum_{k_H k_L} \langle \Psi | \hat{P}_{0,0}^{\Lambda} \hat{P}_{\kappa_H \kappa_H}^{S_H} \hat{P}_{\kappa_L \kappa_L}^{S_L} | \Psi \rangle.$$

$$P(\Lambda, S_H, S_L) = \sum_{K_H K_L K'_H K'_L} (-1)^{K'_H - K_H + K'_L - K_L}$$

$$C^{\Lambda,0}_{S_{H},-\kappa_{H},S_{L},-\kappa_{L}}C^{\Lambda,0}_{S_{H},-\kappa_{H}',S_{L},-\kappa_{L}'}\langle\Psi|\hat{P}^{S_{H}}_{\kappa_{H}\kappa_{H}'}\hat{P}^{S_{L}}_{\kappa_{L}\kappa_{L}'}|\Psi\rangle$$



G.scamps, I. Abdurrahman, M. Kafker, A. Bulgac, and I. Stetcu, PRC 108 (6), L061602.



### Method

- TDHFB TDSLDA
- Full projection beyond one-angle approximation

#### Results

- Distribution of K
- Small fluctuations around the 90 degrees angle
- Almost flat distribution of opening angle

### Limitation

- No collective wave function
- G. Scamps, G. Bertsch, Phys. Rev. C 108, 034616 (2023).



### Question

- How the quantal effects change this picture?
- How the geometry change the opening angle distribution assuming no correlation?

# Non alignement of the spins

To get a 5 degrees angle between two spins require spins of 262  $\hbar$  and 6565  $\hbar$  for 1 degree



$$|\Psi\rangle = \sum_{S_H, \kappa_H, S_L, \kappa_L} c_{S_H, \kappa_H, S_L, \kappa_L} |S_H, \kappa_H, S_L, \kappa_L\rangle,$$

$$\begin{aligned} |c_{S_{H},\kappa_{H},S_{L},\kappa_{L}}|^{2} \propto & \delta_{\kappa_{H},0} \delta_{\kappa_{L},0} (2S_{H}+1) e^{\frac{-S_{H}(S_{H}+1)}{2\sigma_{H}^{2}}} \\ & \times (2S_{L}+1) e^{\frac{-S_{L}(S_{L}+1)}{2\sigma_{L}^{2}}}. \end{aligned}$$



G. Scamps, PRC 109, L011602 (2024).

# Opening angle distribution - 3D uniform case



G. Scamps, PRC 109, L011602 (2024).



# Opening angle distribution - 3D from TDDFT

 $\theta_{\rm F}$  [deg]



### Main points

- Orientation-pumping (uncertainty principle) mechanism at scission
- Additional effect of the Coulomb torque
- Internal excitation (breaking of pairs)
- Spins are mainly perpendicular to the fission axis
- Uncorrelated magnitude and orientation of the spins
- Dependence of the mechanism with the deformation (quadrupole and octupole)

# Outlook : Case where total spin is not zero

 $^{208}Pb + ^{208}Pb$ 



<sup>50</sup>Ca+<sup>176</sup>Yb



G. Scamps, Microscopic Study of Spin Transfer in Near-Barrier Nuclear Reactions, arXiv :2409.15018 (2024).

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# Thank you

# Overdamped motion from saddle point to scission

### TDHF



TDHF+BCS



#### **TDHFB**





Mainly two regimes before and after scission :

1) Overdamped motion, trajectory minimizing the energy

2) Fast separation, the asymmetry of the fission is frozen

### Important

The fission properties are decided at scission

