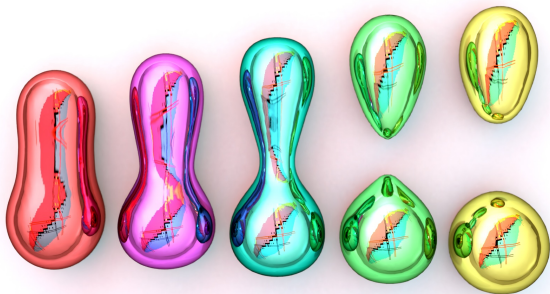


Joint IRN-FenmTo COPIGAL POLITA Workshop

# Generation of fission fragments' spin in microscopic models

Guillaume SCAMPS

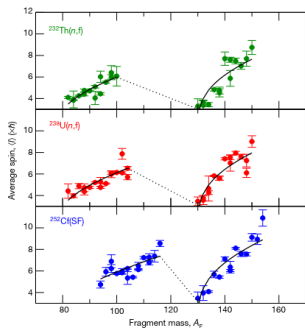


 Université  
de Toulouse

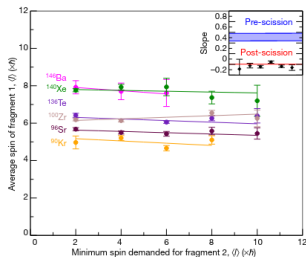
 L2T

 cnrs

## Spin of the fragments



## Correlations



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

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

## Literature

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

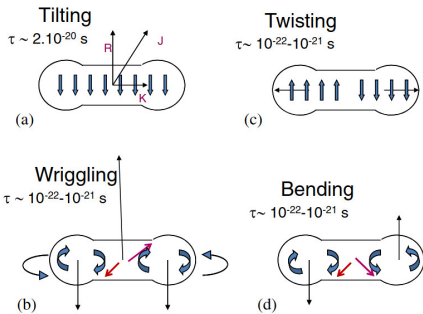
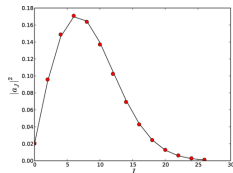


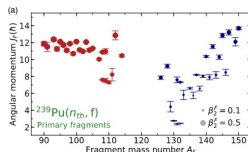
Illustration from B. John, J. Phys., 85, 2, (2015).

## Static HFB



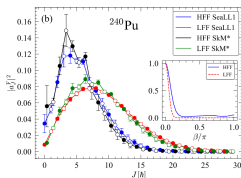
G. F. Bertsch, T. Kawano, and L. M. Robledo,  
PRC 99, 034603 (2019)

## Scission configuration



P. Marević, N. Schunck, J. Randrup, and R.  
Vogt PRC 104, L021601 (2021).

## TDHFB - TDSLDA



A. Bulgac, et al., PRL 126, 142502 (2021)

## Projection method

$$\hat{P}_J (|\Psi(J=0)\rangle + |\Psi(J=1)\rangle + \dots) = |\Psi(J)\rangle$$

$$|a_J^F|^2 = \frac{2J+1}{2} \int_0^{2\pi} \sin(\beta)$$

$$P_J(\cos(\beta)) \langle \Psi | e^{-iJ_x^F \beta / \hbar} | \Psi \rangle$$

## TDHFB equations

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} h(t) & \Delta(t) \\ -\Delta^*(t) & -h^*(t) \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}$$

## TDHFB equations

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} h(t) & \Delta(t) \\ -\Delta^*(t) & -h^*(t) \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}$$

## Strengths

- Self-consistent mean field + pairing
- Functional and no other adjustable parameters.
- One-body dissipation
- Large-amplitude collective motion

## TDHFB equations

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} h(t) & \Delta(t) \\ -\Delta^*(t) & -h^*(t) \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}$$

## Strengths

- Self-consistent mean field + pairing
- Functional and no other adjustable parameters.
- One-body dissipation
- Large-amplitude collective motion

## Limitations

- Missing quantum and statistic fluctuations
- Broken symmetries (projection needed)
- Computationally expensive

### TDHFB equations

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} h(t) & \Delta(t) \\ -\Delta^*(t) & -h^*(t) \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}$$

### TDBCS approximation

Canonical basis evolution :

$$i\hbar \dot{\varphi}_\alpha = h \varphi_\alpha$$

$$i\hbar \dot{n}_\alpha = \kappa_\alpha \Delta_\alpha^* - \kappa_\alpha^* \Delta_\alpha$$

$$i\hbar \dot{\kappa}_\alpha = 2\epsilon_\alpha \kappa_\alpha + \Delta_\alpha (2n_\alpha - 1)$$

### Strengths

- Self-consistent mean field + pairing
- Functional and no other adjustable parameters.
- One-body dissipation
- Large-amplitude collective motion

### Limitations

- Missing quantum and statistic fluctuations
- Broken symmetries (projection needed)
- Computationally expensive

### TDHFB framework

- Gogny-TDHFB code
- Gogny D1S interaction
- Hybrid basis :
  - ▶ 2D harmonic oscillator ( $x, y$ )
  - ▶ 1D spatial mesh ( $z$ )

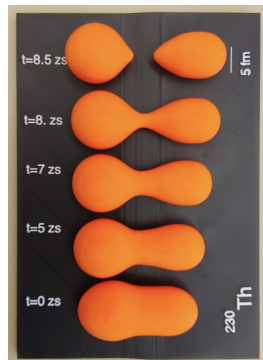
### Numerical setup

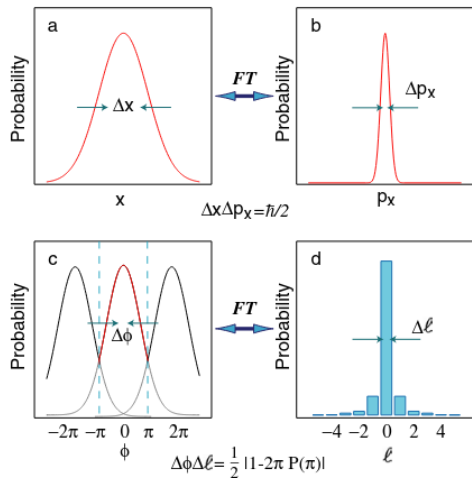
- $\Delta z = 0.8 \text{ fm}$ ,  $N_z = 52$
- $n_x + n_y \leq N_{\text{shell}} = 9$
- $\hbar\omega = 8 \text{ MeV}$
- $\Delta t = 2 \times 10^{-3} \text{ zs}$

### Fissioning nuclei

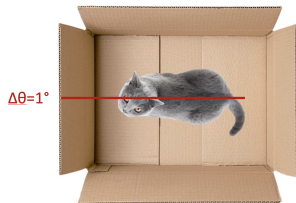
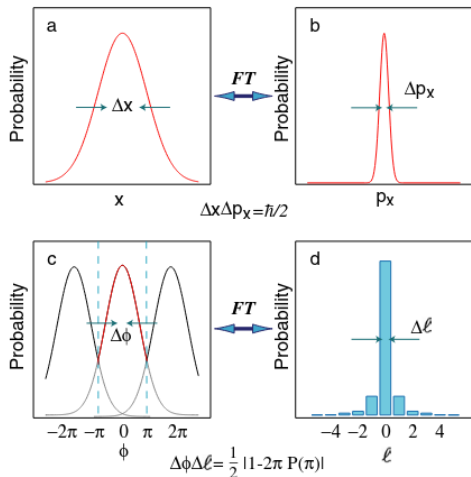
- $^{230}\text{Th}$
- $^{240}\text{Pu}$
- $^{250}\text{Cf}$

Asymmetric fission region  
Heavy fragment influenced by octupole deformation

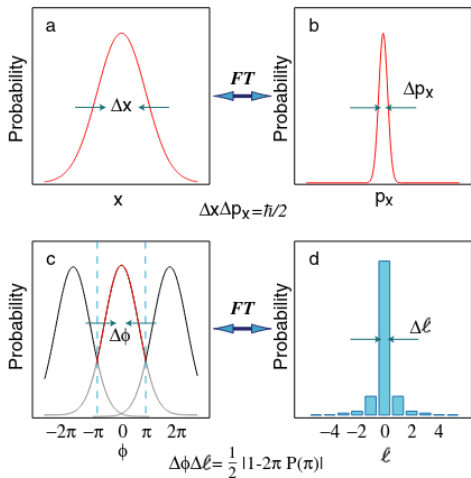




S. Franke-Arnold, et al. New Journal of Physics 6, 103 (2004)



















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



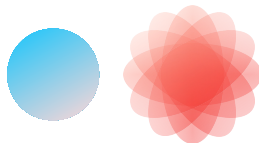
For  $\Delta\Theta = 1^\circ$ ,  $\Delta L = 29\hbar$ .  
 For a cat, angular velocity  
 $\omega = 10^{-33} \text{ s}^{-1}$

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

Premiers harmoniques sphériques

	$m = -3$	$m = -2$	$m = -1$	$m = 0$	$m = +1$	$m = +2$	$m = +3$
$l = 0$				$\frac{1}{\sqrt{4\pi}}$ 			
$l = 1$			$\frac{1}{\sqrt{4\pi}} \sqrt{\frac{3}{2}} \sin \theta e^{-i\phi}$ 	$\frac{1}{\sqrt{4\pi}} \sqrt{3} \cos \theta$ 	$\frac{1}{\sqrt{4\pi}} \sqrt{\frac{3}{2}} \sin \theta e^{i\phi}$ 		
$l = 2$		$\frac{1}{\sqrt{4\pi}} \sqrt{\frac{15}{8}} \sin^2 \theta e^{-i2\phi}$ 	$\frac{1}{\sqrt{4\pi}} \sqrt{\frac{15}{2}} \cos \theta \sin \theta e^{-i\phi}$ 	$\frac{1}{\sqrt{4\pi}} \sqrt{\frac{5}{2}} (3 \cos^2 \theta - 1)$ 	$\frac{1}{\sqrt{4\pi}} \sqrt{\frac{15}{2}} \cos \theta \sin \theta e^{i\phi}$ 	$\frac{1}{\sqrt{4\pi}} \sqrt{\frac{15}{8}} \sin^2 \theta e^{i2\phi}$ 	
$l = 3$							

## Orientation pumping mechanism

Isotropic potential at scissionConfining potential at scission

L. Bonneau, P. Quentin, and I. N. Mikhailov, PRC 75, 064313 (2007).

For  $\Delta\Theta = 1^\circ$ ,  $\Delta L = 29\hbar$ .

For a nucleus, angular velocity

$$\omega = 10^{20} \text{ s}^{-1}$$

### Conceptual difficulty

- Unlike position, angular variables are **periodic**.
- Mean values and fluctuations of an angle are not uniquely defined.
- Restrict to well-oriented wave packet

### Orientation–angular momentum uncertainty

$$\Delta\theta \Delta L_x > \frac{1}{2}, \quad (L_x \text{ in units of } \hbar)$$

Analogous relation for  $L_y$ .

### Gaussian orientation state and spin distribution

Gaussian wave packet :

$$\Psi(\theta, \varphi) = \mathcal{N} \exp\left[-\frac{\theta^2}{4\sigma_\theta^2}\right]$$

Spin cut-off distribution :

$$P(L) = \frac{2L+1}{\mathcal{Z}} \exp\left[-\frac{L(L+1)}{2\sigma_L^2}\right]$$

Heisenberg-type relation :

$$\sigma_\theta \sigma_L = \frac{1}{2}$$

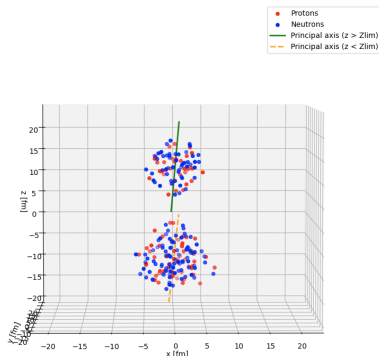
## Second difficulty : composite nuclei

- In collective Hamiltonian models, angle wave packets are well defined.
- In microscopic approaches, orientation is **not an operator**.
- No direct definition of angular fluctuations.

## Proposed approach

- Go beyond the one-body density picture.
- Sample nucleon positions and intrinsic spins from the Bogoliubov vacuum.
- Markov Chain Monte Carlo sampling (NucleoScope).
- Determine principal axis event-by-event.

## Principal axis determination



Examples for  $^{230}\text{Th}$ .  
 Red/blue dots : proton/neutron distributions.  
 Lines : fragment principal axes.

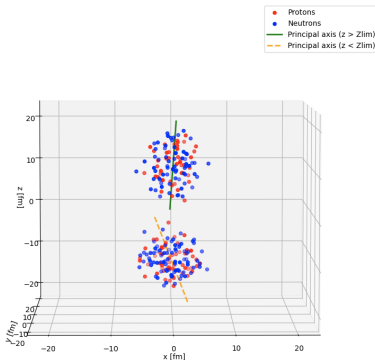
## Second difficulty : composite nuclei

- In collective Hamiltonian models, angle wave packets are well defined.
- In microscopic approaches, orientation is **not an operator**.
- No direct definition of angular fluctuations.

## Proposed approach

- Go beyond the one-body density picture.
- Sample nucleon positions and intrinsic spins from the Bogoliubov vacuum.
- Markov Chain Monte Carlo sampling (NucleoScope).
- Determine principal axis event-by-event.

## Principal axis determination



Examples for  $^{230}\text{Th}$ .  
 Red/blue dots : proton/neutron distributions.  
 Lines : fragment principal axes.

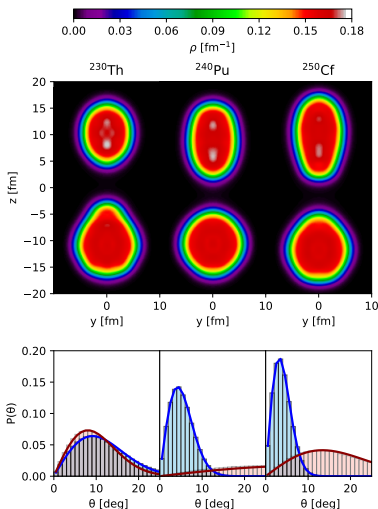
Distribution of  $\theta$ 

- For each sampled event, principal axis of each fragment is computed.
- Obtain  $\theta$  = angle between fragment axis and global z-axis.
- Construct full probability distribution  $P(\theta)$ .
- Expectation value  $\langle \theta \rangle = 0$  due to symmetry.
- Standard deviation  $\sigma_\theta$  characterizes the angular fluctuation.

## Physical meaning

- Reflects uncertainty in fragment orientation.
- Geometric definition mainly sensitive to quadrupole deformation.
- Can be used for spin-cutoff estimations.

## Angular distribution figure



Angular distribution  $P(\theta)$  for light (blue) and heavy (red) fragments. Fitted curves illustrate approximate Gaussian behavior.

## Angular distribution

$$f(\theta) = \mathcal{N}^2 \sin(\theta) \exp \left[ -\frac{\theta^2}{2\sigma_\theta^2} \right]$$

- Excellent agreement with Gaussian form
- Angular fluctuations are Gaussian
- Larger quadrupole deformation  $\Rightarrow$  narrower distribution

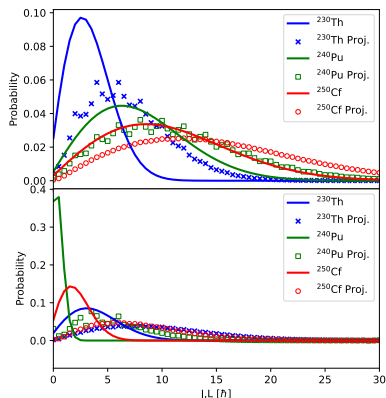
From  $\sigma_\theta$  to spin

$$\sigma_\theta \sigma_L = \frac{1}{2}$$

- Extract  $\sigma_\theta$
- Deduce spin cut-off  $\sigma_L$
- Build spin distribution

## Spin distribution

$$P(L) = \frac{2L+1}{\mathcal{Z}} \exp \left[ -\frac{L(L+1)}{2\sigma_L^2} \right]$$



Projection results vs. spin cut-off formula (light : top, heavy : bottom).

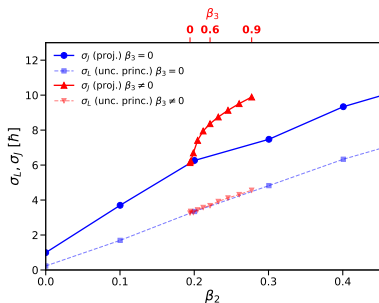
### Microscopic vs geometric picture

- Exact angular momentum obtained from projection of many-body states.
- Monte Carlo sampling determine the fluctuations of the fragment principal axis from  $Q_2$  deformation.

### Octupole deformation

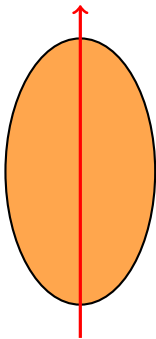
- Principal axis distribution becomes flat.
- Geometric picture underestimates spin.

### Spin-cutoff vs deformation



Spin cut-off parameter for  $^{144}\text{Ba}$ . Solid lines : projection. Dashed lines : principal-axis uncertainty estimate.

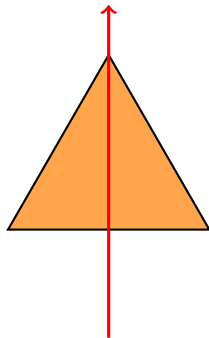
## Prolate deformation



$$Q_2 > 0$$

Principal axis well defined

## Triangular (octupole) configuration



$$Q_2 = 0$$

Orientation still defined but principal axis isotropic

## Overlap of rotated many-body states

$$\langle \Psi | e^{i\alpha \hat{J}_z} e^{i\theta \hat{J}_y} e^{i\gamma \hat{J}_z} | \Psi \rangle \simeq \exp \left[ -\frac{\theta^2}{8\sigma_\theta^2} \right]$$

- Gaussian approximation for small rotations
- Width  $\sigma_\theta$  characterizes angular localization

## Physical meaning

- Many-body state localized in rotational space
- Does **not** rely on geometric definition of orientation
- Orientation angle and angular momentum are conjugate variables

## Spin fluctuations

Spin cut-off distribution :

$$P(J) = \frac{2J+1}{\mathcal{Z}} \exp \left[ -\frac{J(J+1)}{2\sigma_J^2} \right]$$

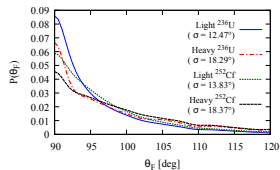
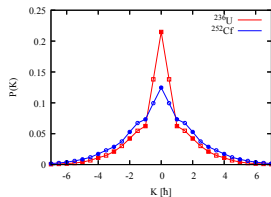
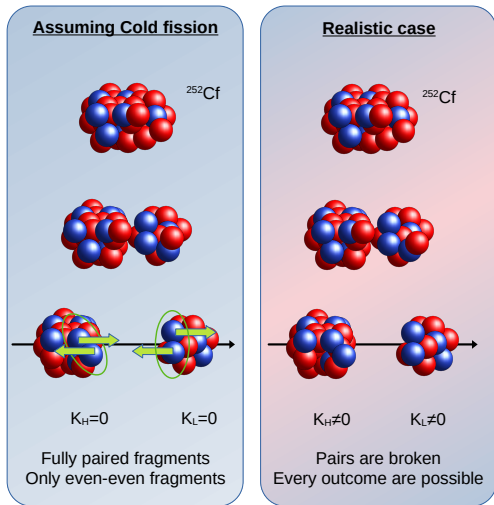
$$\sigma_\theta \sigma_J = \frac{1}{2}$$

Nucleus	Frag.	$\sigma_L$	$\sigma_J$	$\sigma_J$
		(uncert. with principal axis)	(overlap)	(projection)
$^{230}\text{Th}$	L	2.90	5.74	5.81
	H	3.37	7.84	7.88
$^{240}\text{Pu}$	L	6.79	9.32	9.37
	H	0.75	4.67	4.93
$^{250}\text{Cf}$	L	9.00	12.18	12.27
	H	2.12	6.50	6.63

## Key result

- Spin cut-off parameters extracted from :
  - ▶ angular fluctuations + uncertainty relation
  - ▶ Gaussian overlap fit
  - ▶ exact angular-momentum projection
- **Excellent agreement** between overlap and exact projection.
- Error with the principal axis method (miss higher order deformation).

G. Scamps, A. Guilleux, D. Regnier, A. Bernard, Uncertainty Principle and Angular Momentum Generation in Microscopic Fission Models, arXiv :2512.02207 [nucl-th].



$$\cos \theta_F = \frac{K_F}{\sqrt{S_F(S_F + 1)}}$$

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

$^{144}\text{Ba} + ^{96}\text{Sr}$  at 16 Fm,  $\Theta_{ini}=25$  deg, Functional : Skyrme Sly4d

$J_y(x, z)[\hbar \text{ fm}^{-3}]$

G. Scamps, PRC 106, 054614 (2022).

One body-evolution - One body-observable

$^{144}\text{Ba} + ^{96}\text{Sr}$  at 16 Fm,  $\Theta_{ini}=25$  deg, Functional : Skyrme Sly4d

$J_y(x, z)[\hbar \text{ fm}^{-3}]$

G. Scamps, PRC 106, 054614 (2022).

One body-evolution - One body-observable

$^{144}\text{Ba} + ^{96}\text{Sr}$  at 16 Fm,  $\Theta_{ini}=25$  deg, Functional : Skyrme Sly4d

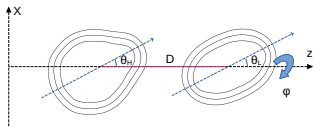
$J_y(x, z)[\hbar \text{ fm}^{-3}]$

G. Scamps, PRC 106, 054614 (2022).

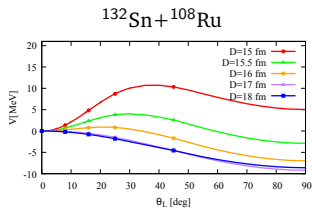
$^{144}\text{Ba} + ^{96}\text{Sr}$  at 16 Fm,  $\Theta_{ini}=25$  deg, Functional : Skyrme Sly4d

$J_y(x, z)[\hbar \text{ fm}^{-3}]$

G. Scamps, PRC 106, 054614 (2022).



## Potential as a function of the light fragment angle

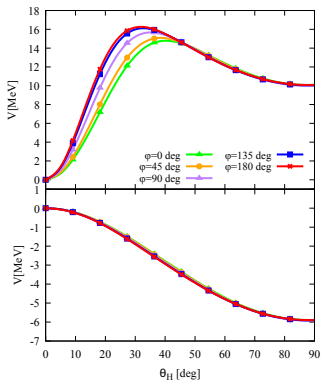


Two torques :

- attractive nucleus-nucleus torque
- repulsive Coulomb torque

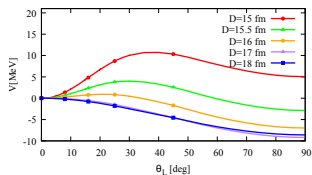
## Potential as a function of the light fragment angle

$^{144}\text{Ba} + ^{96}\text{Sr}$ .  $D=15.5$  and  $20$  fm



The azimuthal angle doesn't have an important role.

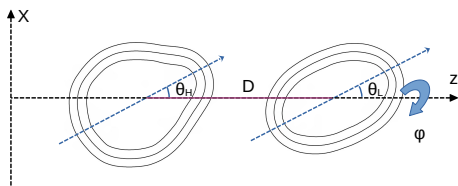
## Frozen Hartree-Fock potential



Two torques :

- attractive nucleus-nucleus torque
- repulsive Coulomb torque

## 4 degrees of freedom



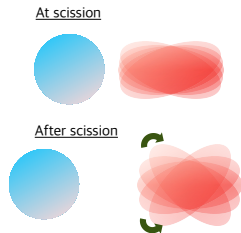
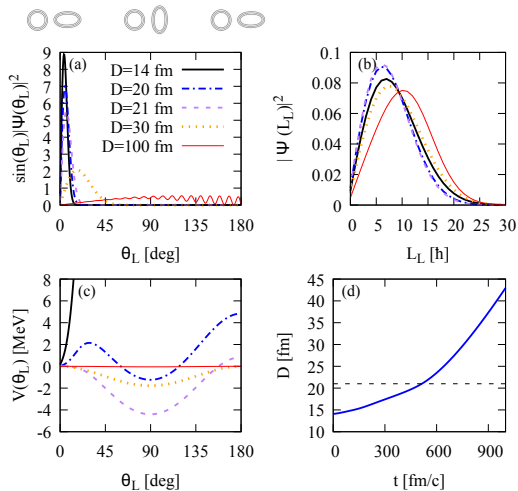
## Hamiltonian

$$\hat{H}(D) = \frac{\hbar^2}{2I_H} \hat{L}_H^2 + \frac{\hbar^2}{2I_L} \hat{L}_L^2 + \frac{\hbar^2}{2I_\Lambda(D)} \hat{\Lambda}^2 + \hat{V}(\hat{\Theta}_H, \hat{\Theta}_L, \hat{\varphi}, D)$$

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. Physics Letters B, 462(1-2), 7-13 (1999)



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

### Theoretical tools

- Development of advanced TDDFT approaches with projection techniques and position sampling
- Frozen Hartree-Fock
- Collective Hamiltonian approaches for quantum collective motion

### Mechanism for the generation of fragment spin

- Coulomb interaction at scission tends to deform the fragments
- Fragments are oriented along the fission axis
- The uncertainty principle induces angular momentum

Thank you for your attention