Demystifying the fusion mechanism in heavy ion collisions within full Langevin dissipative dynamics

Yannen Jaganathen, Michał Kowal, Krzysztof Pomorski (NCBJ, Warsaw)

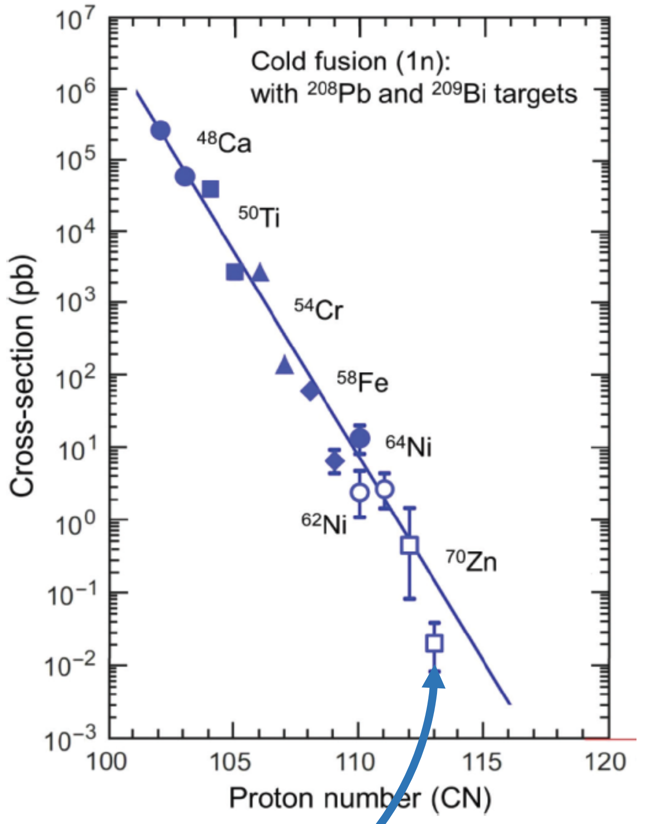
Based on: *Phys. Lett. B 862 (2025) 139302*

Description of the fusion mechanism within Langevin dynamics

Super-heavy elements with Z > 103 do not occur in nature.
They can only be produced in the laboratory by fusing two lighter nuclei.

Our primary goal is to gain insights into the **fusion reaction mechanisms in the domain of cold synthesis reactions** ($Z < 113$, $E^* \approx 10 - 20$ MeV), in particular on the **understanding of the hindrance mechanism which prevents the formation of super-heavy nuclei.**

We propose a comprehensive dissipative dynamics **Langevin**-based formalism to describe the unrestricted motion of the systems in terms of **elongation**, **neck** and **asymmetry** variables.



Z = 113, 22fb
(Only 3 atoms in
576 days of irradiation)

Credits: T. Cap, M. Kowal

Plan

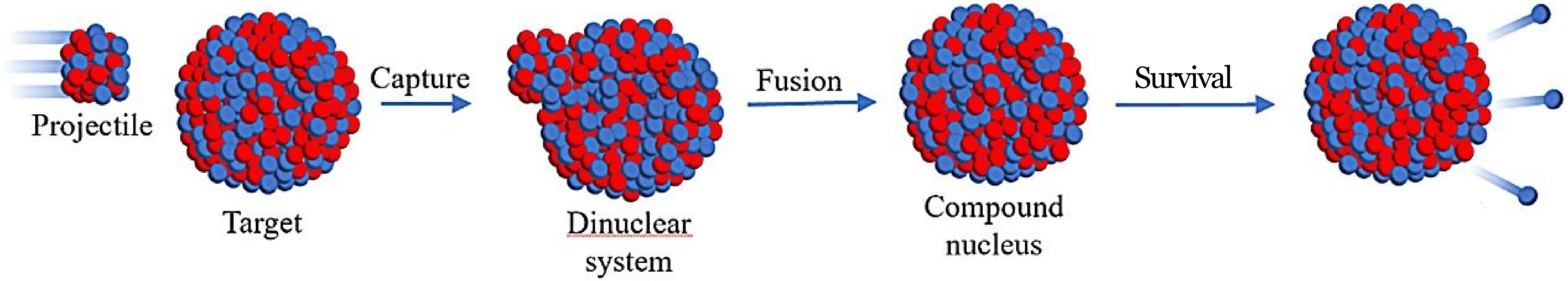
1. The **Ingredients** of the Langevin Formalism
   - The **Potential**
   - The **Mass Tensor**
   - The **Friction Forces**
   - The **Langevin/Random Force** and Its Origin
   - The Calculated **Observables**

2. The Langevin Formalism and the **Fusion Mechanism in Heavy-Ion Collisions**

3. **Applications**

4. **Summary and Perspectives**

The fusion process (Schematic view)



Micro-macroscopic description of fusion:

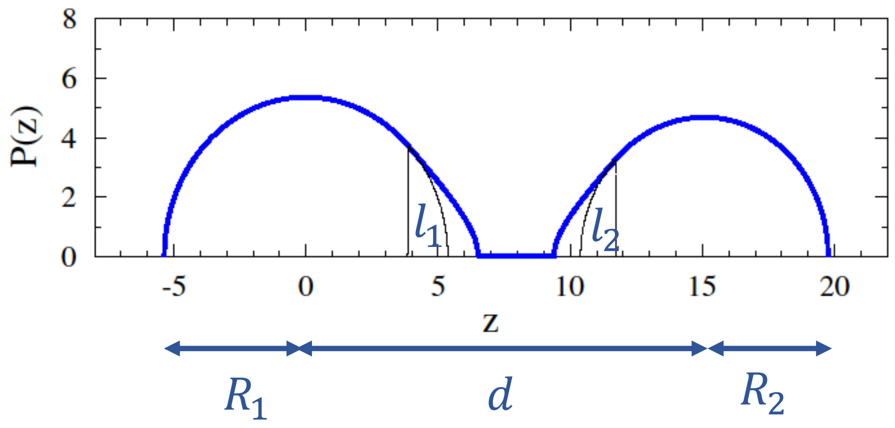
- Complexity/impossibility of tracking all internal degrees of freedom
- Identification of **slow collective degrees of freedom** immersed in a **bath** of faster dynamics
- Emergence of the mechanisms of **friction** and **random forces**
- Macroscopic model with some microscopic corrections.

Collective variables adapted to fusion/fission – Shape variables

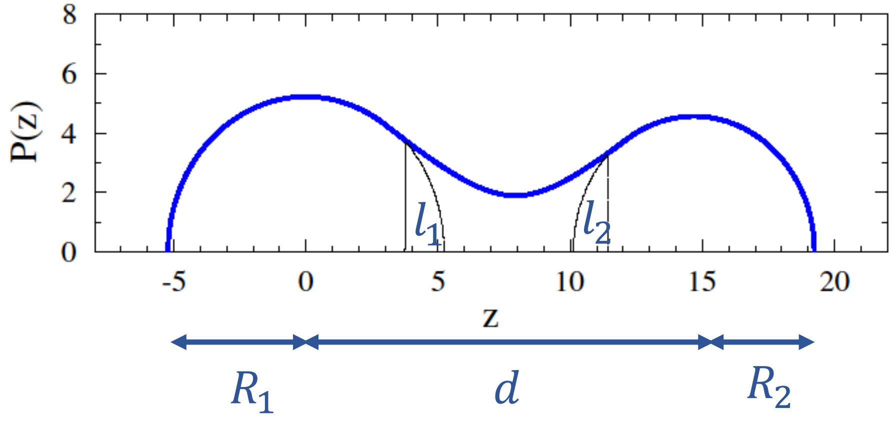
- Axially symmetric shapes
- **Spherical** cups connected by quadratic surfaces[1]

- **Shape collective/slow variables**:
  - **Distance/elongation** : $\rho = \frac{d}{R_1+R_2}$
  - **Neck/deformation** : $\lambda = \frac{l_1+l_2}{R_1+R_2}$
  - **Asymmetry**: $\Delta = \frac{R_1-R_2}{R_1+R_2}$

$^{92}Zr + ^{64}Ni$



Bipartite
$\rho = 1.5$
$\lambda = 0.3$
$\Delta = \Delta_0$



Monopartite
$\rho = 1.5$
$\lambda = 0.4$
$\Delta = \Delta_0$

[1] J. Błocki, H. Feldmeier and W. J. Świątecki, Nucl. Phys. A 459 (1986) 145

Collective variables adapted to fusion/fission – Shape variables

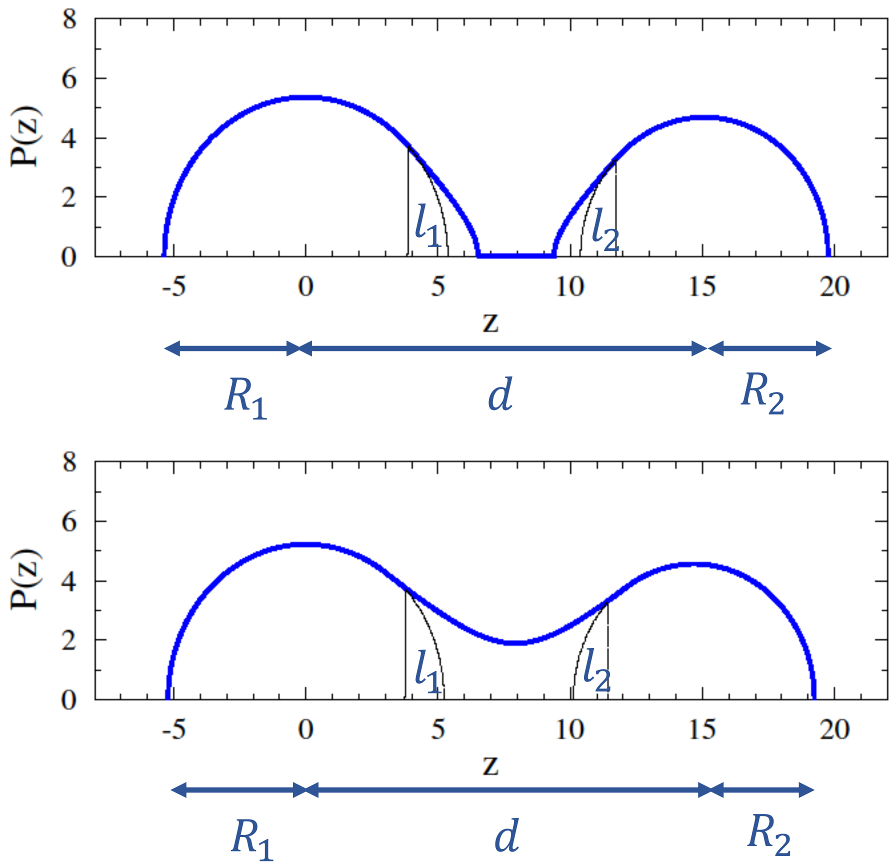
- Axially symmetric shapes
- **Spherical** cups connected by quadratic surfaces[1]

- **Shape collective/slow variables**:
  - **Distance/elongation** : $\rho = \frac{d}{R_1+R_2}$
  - **Neck/deformation** : $\lambda = \frac{l_1+l_2}{R_1+R_2}$
  - **Asymmetry**: $\Delta = \frac{R_1-R_2}{R_1+R_2}$

- **Scission is well-defined**: $\lambda_{\text{scission}} = 1 - \frac{1}{\rho_{\text{scission}}}$

  $\longrightarrow$ **Suited to describe fusion/fission** (vs. multipole moments)

$^{92}Zr + ^{64}Ni$



Bipartite
$\rho = 1.5$
$\lambda = 0.3$
$\Delta = \Delta_0$

Monopartite
$\rho = 1.5$
$\lambda = 0.4$
$\Delta = \Delta_0$

[1] J. Błocki, H. Feldmeier and W. J. Świątecki, Nucl. Phys. A 459 (1986) 145

Collective variables adapted to fusion/fission – Angle variables

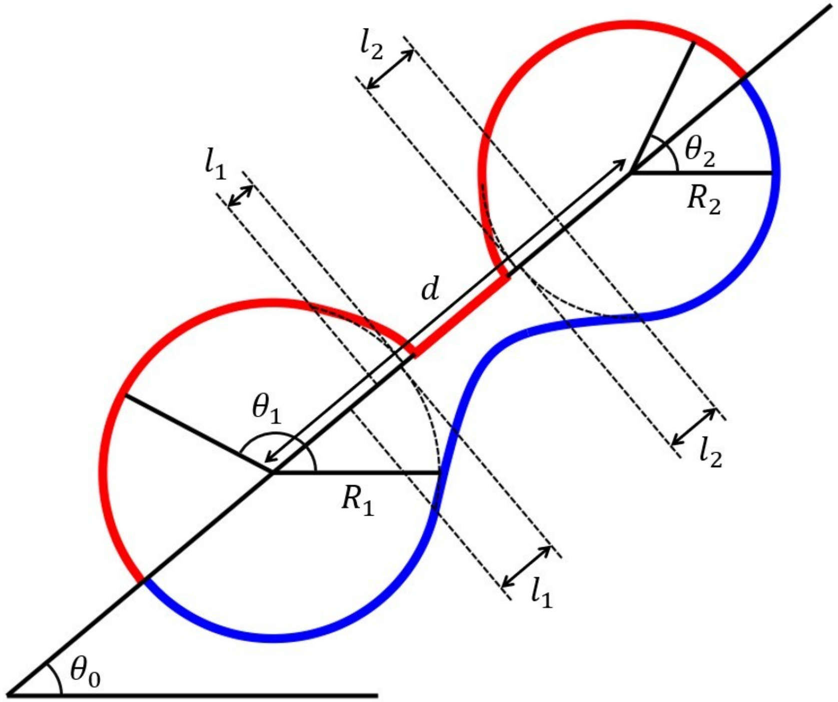
- **Collective angle variables**
  - Angle of the whole system θ_0
  - Angle of the first sphere θ_1
  - Angle of the second sphere θ_2

- Variations linked to angular momentum, in particular:

$$p_{\theta_0} + p_{\theta_1} + p_{\theta_2} = L_{init}$$

- **Exact treatment of angular momentum**

→ **Full Langevin 6-dimensional dissipative dynamics**



The Langevin system of equations

- Denoting **collective/slow variables** $q_i(t)$ and their **associated moments** $p_i(t)$, the **Langevin equations** read:

$$\dot{q}_i(t) = \sum_k (\mathcal{M}^{-1})_{ik}\, p_k \qquad \leftrightarrow (P = MV)$$

$$\dot{p}_i(t) = -\frac{\partial H}{\partial q_i} - \sum_k \gamma_{ik}\, \dot{q}_k + \sum_k g_{ik}\, \xi_k(t) \qquad \leftrightarrow \left(\frac{dP}{dt} = \sum F\right)$$

The Langevin system of equations

- Denoting **collective/slow variables** $q_i(t)$ and their **associated moments** $p_i(t)$, the **Langevin equations** read:

Mass tensor

$$\dot{q}_i(t) = \sum_k (\mathcal{M}^{-1})_{ik}\, p_k \qquad \leftrightarrow (P = MV)$$

$$\dot{p}_i(t) = -\frac{\partial H}{\partial q_i} - \sum_k \gamma_{ik}\, \dot{q}_k + \sum_k g_{ik}\, \xi_k(t) \qquad \leftrightarrow \left(\frac{dP}{dt} = \sum F\right)$$

Conservative forces $(\boldsymbol{H} = \boldsymbol{T} + \boldsymbol{V})$

Friction forces

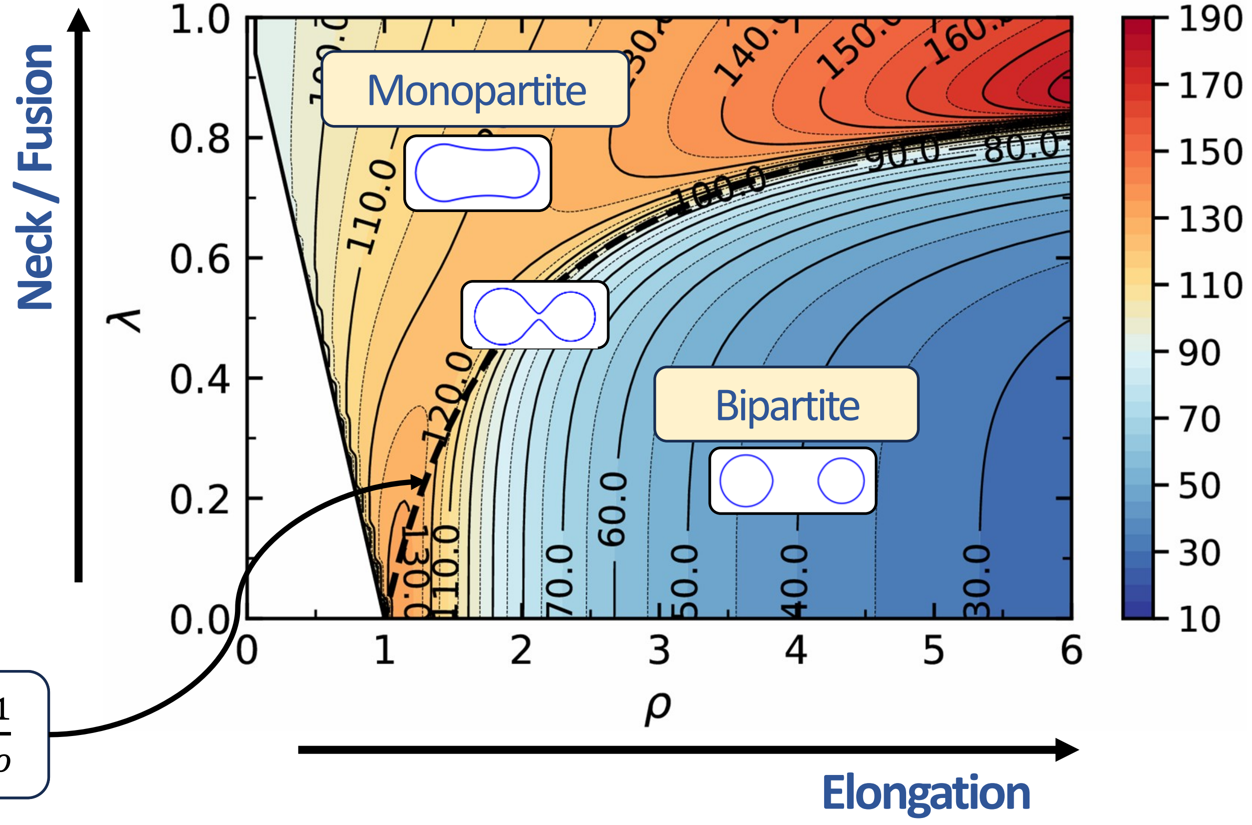
Langevin/random forces

→ A **comprehensive understanding of the dynamics process** (in comparison to the random walk f. eg.).

Collective Potential Energy

- **Yukawa-plus-exponential folding potential + Coulomb**
- Parameters taken from a previous fit to experimental masses and fusion barrier heights [1]
- No shell effects at the moment.

Scission line $\lambda = 1 - \frac{1}{\rho}$

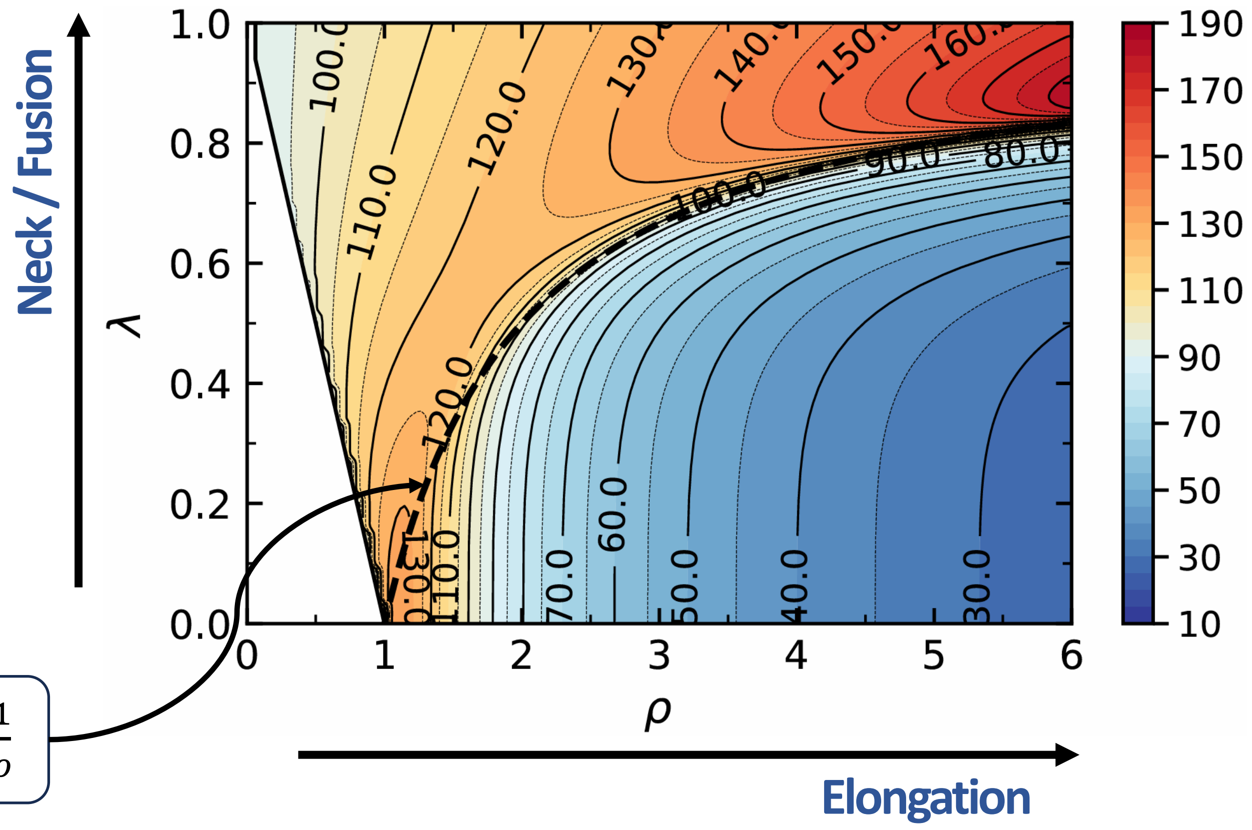


Collective deformation potential of ^{92}Zr + ^{64}Ni in MeV

[1] H. J. Krappe *et al.*, Phys. Rev. C 20 (1979) 992–1013

Collective Potential Energy

- **Yukawa-plus-exponential folding potential + Coulomb**
- Parameters taken from a previous fit to experimental masses and fusion barrier heights [1]
- No shell effects at the moment.



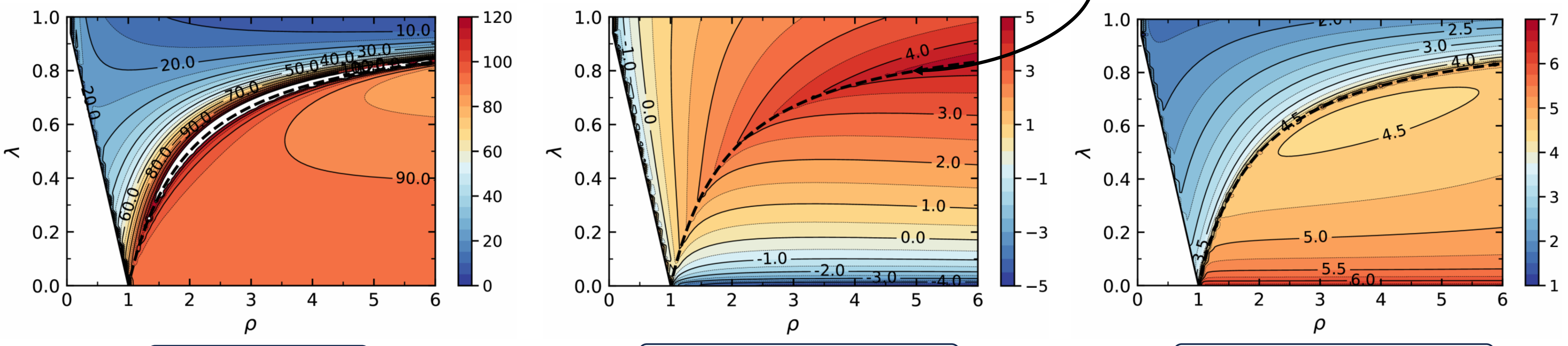
Scission line $\lambda = 1 - \frac{1}{\rho}$

Collective deformation potential of $^{92}Zr + ^{64}Ni$ in MeV

[1] H. J. Krappe *et al.*, Phys. Rev. C 20 (1979) 992–1013

Mass tensor / Kinetic Energy

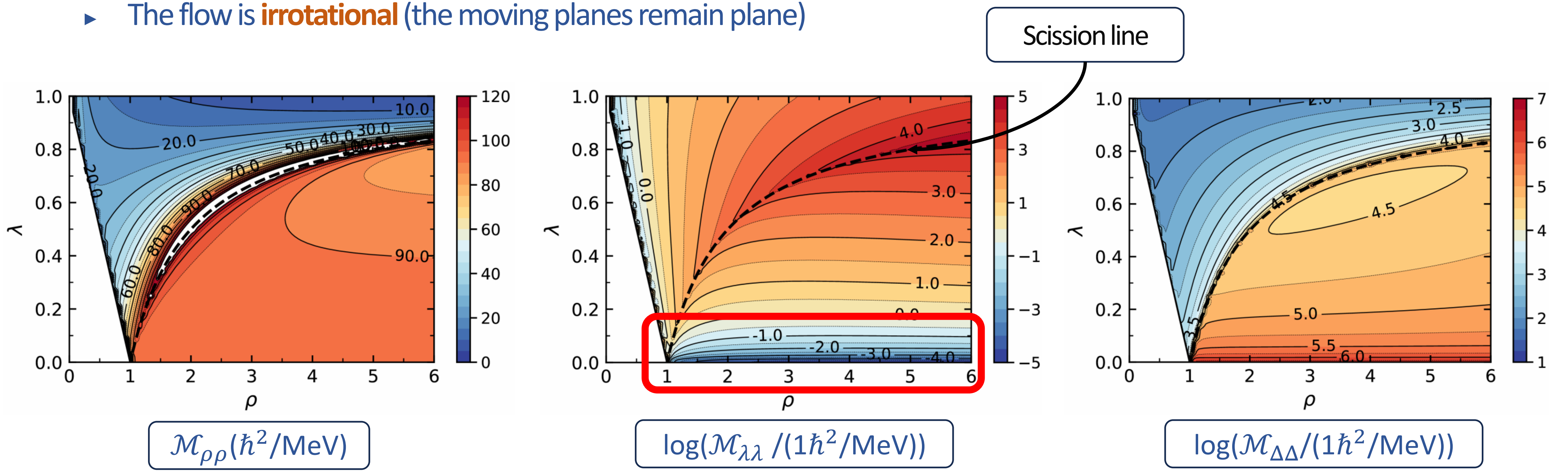
- **Werner-Wheeler flow approximation**:
  - **Incompressibility** (matter density is uniformly distributed)
  - The flow is **irrotational** (the moving planes remain plane)



$\mathcal{M}_{\rho\rho}(\hbar^2/\text{MeV})$ | $\log(\mathcal{M}_{\lambda\lambda}\ /(1\hbar^2/\text{MeV}))$ | $\log(\mathcal{M}_{\Delta\Delta}/(1\hbar^2/\text{MeV}))$

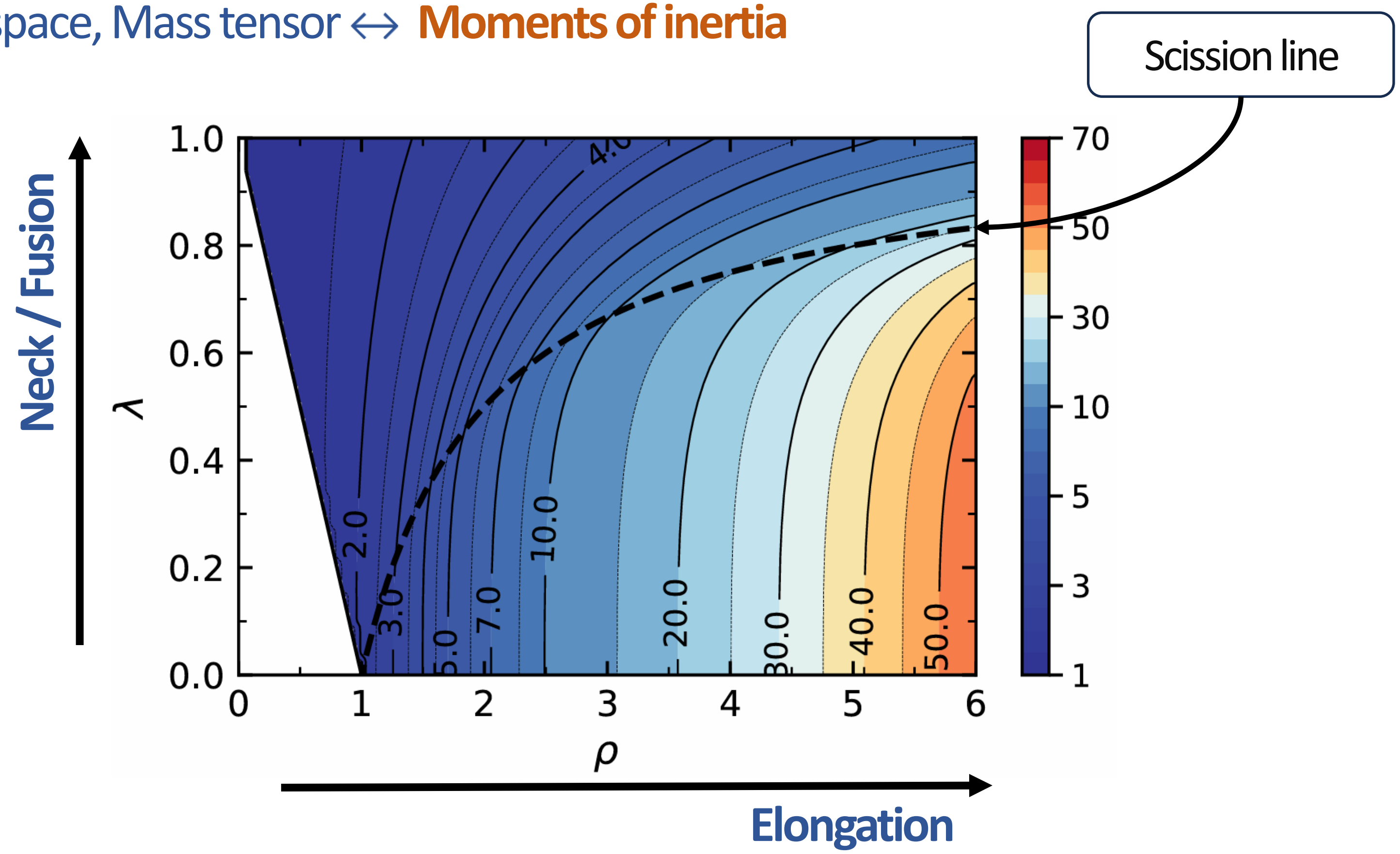
Mass tensor / Kinetic Energy

- **Werner-Wheeler flow approximation**:
  - **Incompressibility** (matter density is uniformly distributed)
  - The flow is **irrotational** (the moving planes remain plane)



Mass tensor / Kinetic Energy

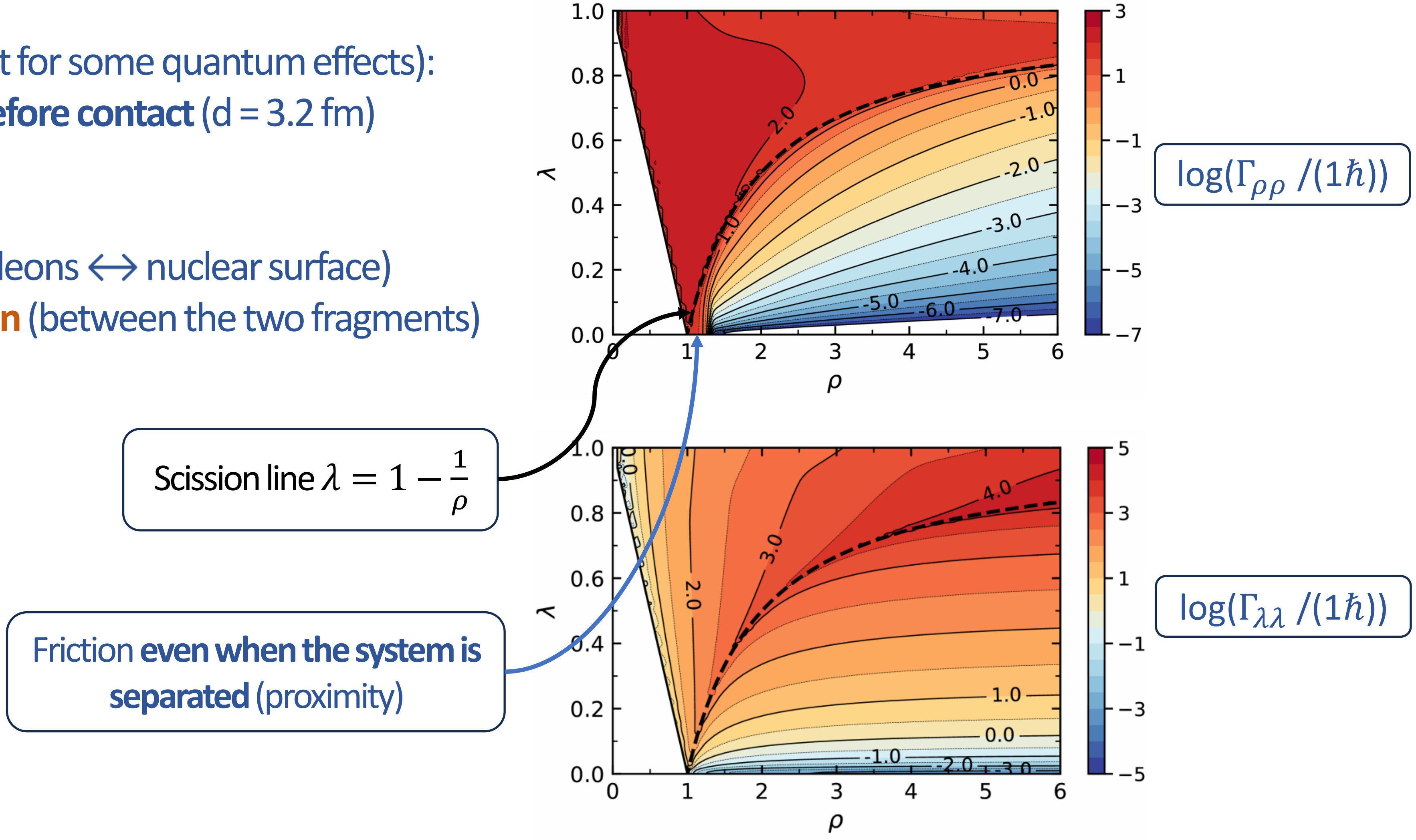
- In the rotational space, Mass tensor ↔ **Moments of inertia**



$I_{tot} \, / \, I_{tot}^{sph}$

Friction forces

- **Proximity formalism** (to account for some quantum effects): **Possible matter flow/friction before contact** (d = 3.2 fm)
- **Shape friction**:
  - **Wall friction** (collisions nucleons ⟷ nuclear surface)
  - + **Wall-plus-window friction** (between the two fragments)

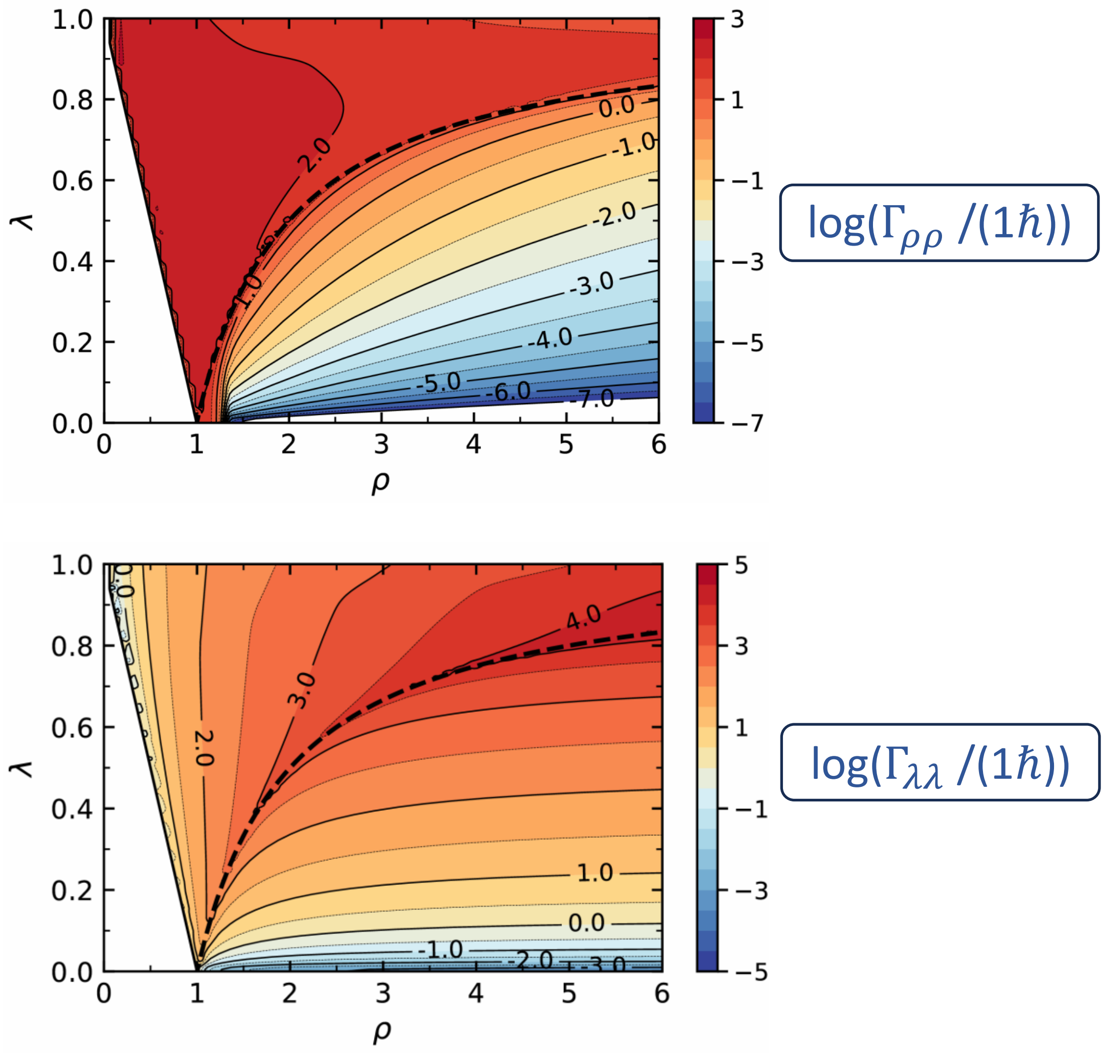


Friction forces

- **Proximity formalism** (to account for some quantum effects):
  Possible matter flow/friction before contact (d = 3.2 fm)

- **Shape friction**:
  - **Wall friction** (collisions nucleons ↔ nuclear surface)
  - + **Wall-plus-window friction** (between the two fragments)

- **Strong friction at the scission line**:
  - **The system slows down at the scission line**
  - **Re-separation is irreversible**



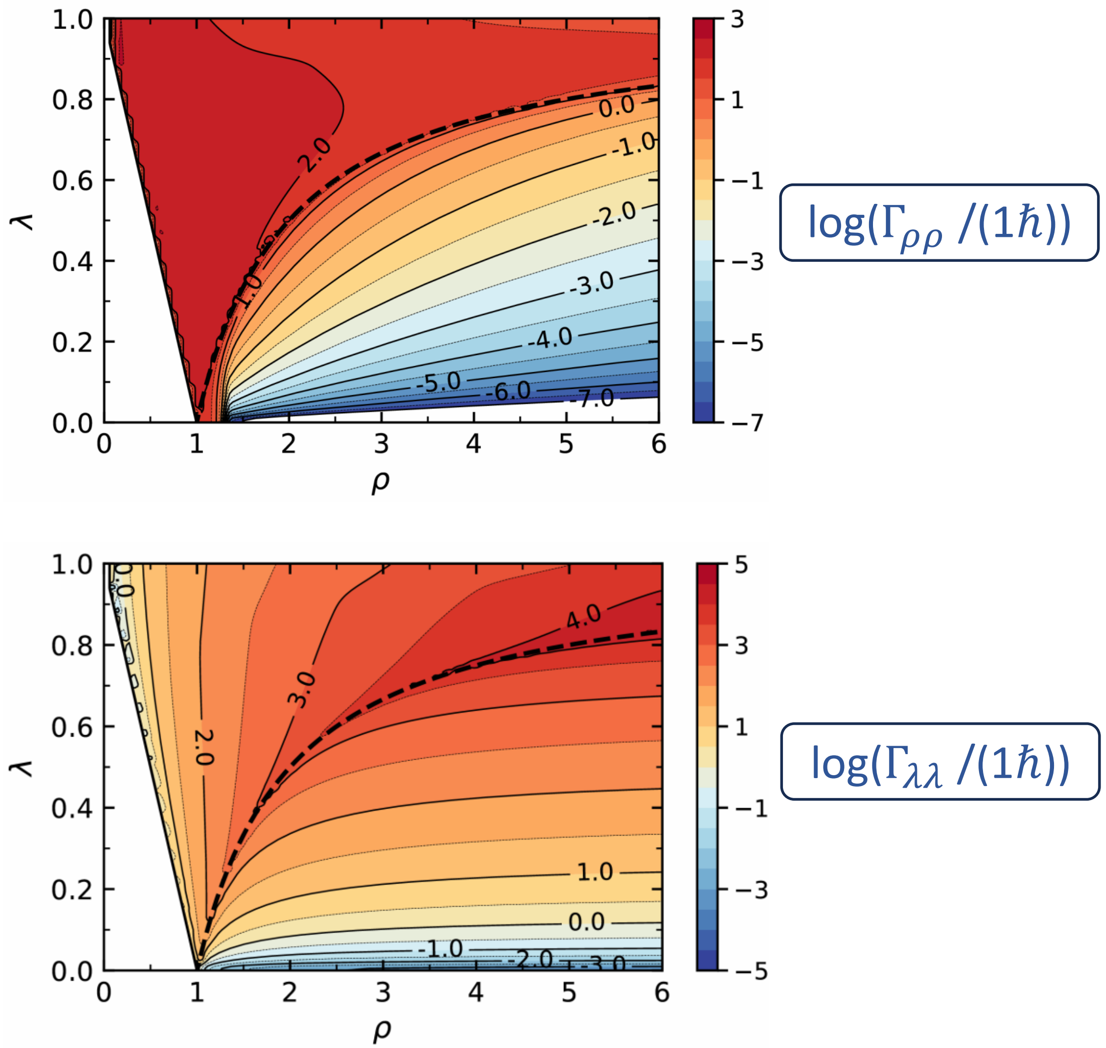
Friction forces

- **Proximity formalism** (to account for some quantum effects):
  Possible matter flow/friction before contact (d = 3.2 fm)

- **Shape friction**:
  - **Wall friction** (collisions nucleons ⟷ nuclear surface)
  - + **Wall-plus-window friction** (between the two fragments)

- **Strong friction at the scission line**:
  - **The system slows down at the scission line**
  - **Re-separation is irreversible**

- **Angular friction**:
  - **Sliding friction**
  - **No rolling friction**



Langevin/random forces

- We assume a simple memoryless Langevin force (white noise):

$$F_i = \sum_k g_{ik}\xi_k(t)$$

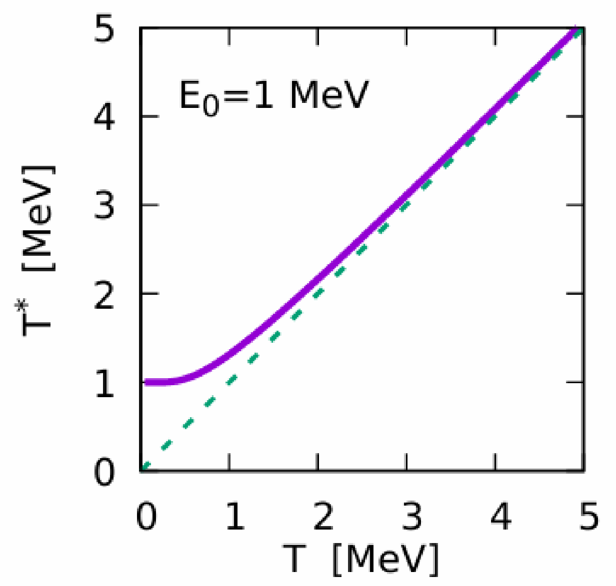
$\xi_k(t)$ are **time-dependent Gaussian random variables:**

$$\langle \xi_k(t) \rangle = 0$$
$$\langle \xi_k(t), \xi_{k'}(t') \rangle = 2\delta_{kk'}\delta(t - t')$$

- The diffusion tensor is given by the **Einstein relation**:

$$\sum_k g_{ik}g_{kj} = D_{ij} = k_B T^* \gamma_{ij}, \qquad T^* = \frac{E_0}{\tanh(E_0/T)}, \qquad T = \sqrt{E^*/a}$$

$E_0 = 2$ MeV is the zero-point collective energy of the heat bath oscillators
E^* is the **dissipated energy**, $a = A/8$ MeV is the **level density parameter**.



Quantum-corrected temperature
(Courtesy of K. Pomorski)

Langevin/random forces

- We assume a simple memoryless Langevin force (white noise):

$$F_i = \sum_k g_{ik} \xi_k(t)$$

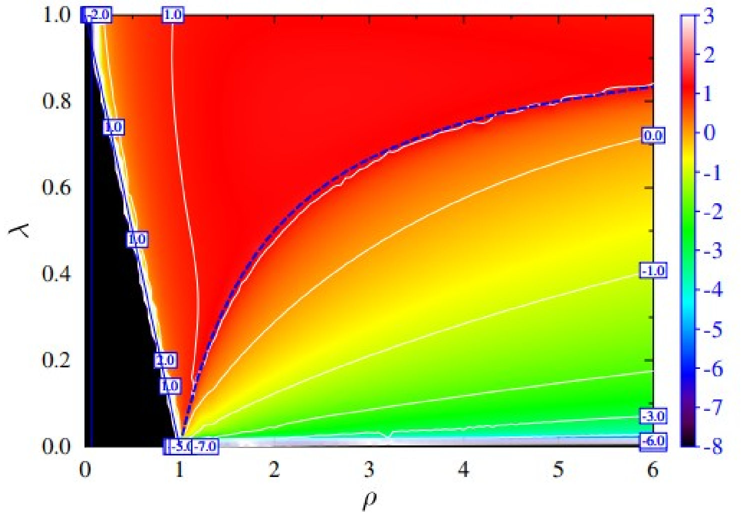
$\xi_k(t)$ are **time-dependent Gaussian random variables:**

$$\langle \xi_k(t) \rangle = 0$$
$$\langle \xi_k(t), \xi_{k'}(t') \rangle = 2\delta_{kk'}\delta(t - t')$$

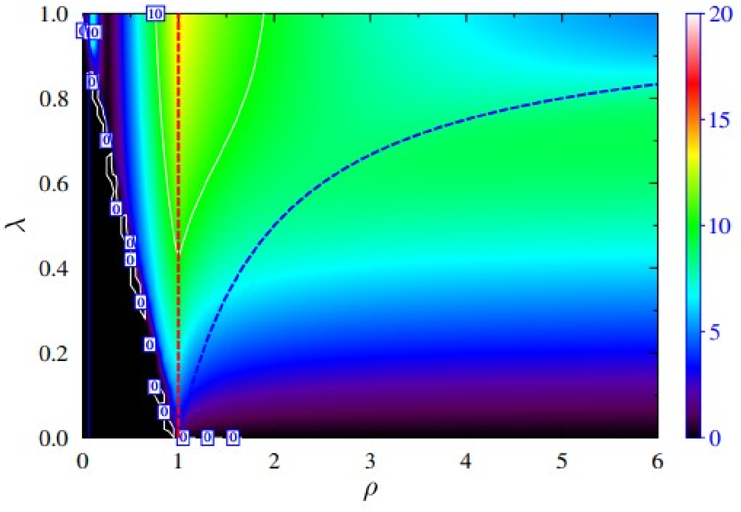
- The diffusion tensor is given by the **Einstein relation**:

$$\sum_k g_{ik} g_{kj} = D_{ij} = k_B T^* \gamma_{ij}\,, \qquad T^* = \frac{E_0}{\tanh(E_0/T)}, \qquad T = \sqrt{E^*/a}$$

$E_0 = 2$ MeV is the zero-point collective energy of the heat bath oscillators
E^* is the **dissipated energy**, $a = A/8$ MeV is the **level density parameter**.



$\log(\hat{g}_{\rho\lambda})$

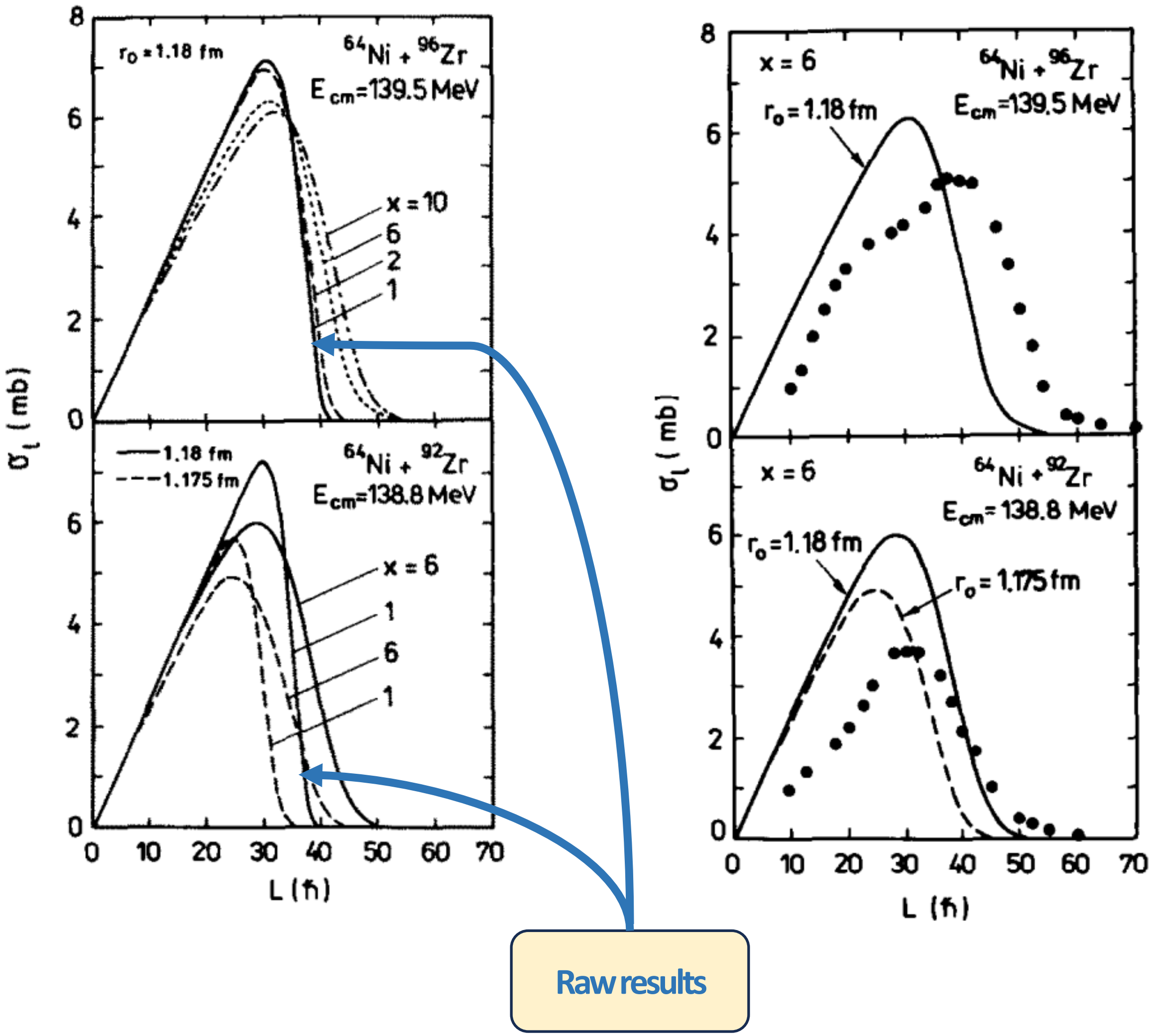


$g_{\theta_2\theta_2}$

A 30 year-old project

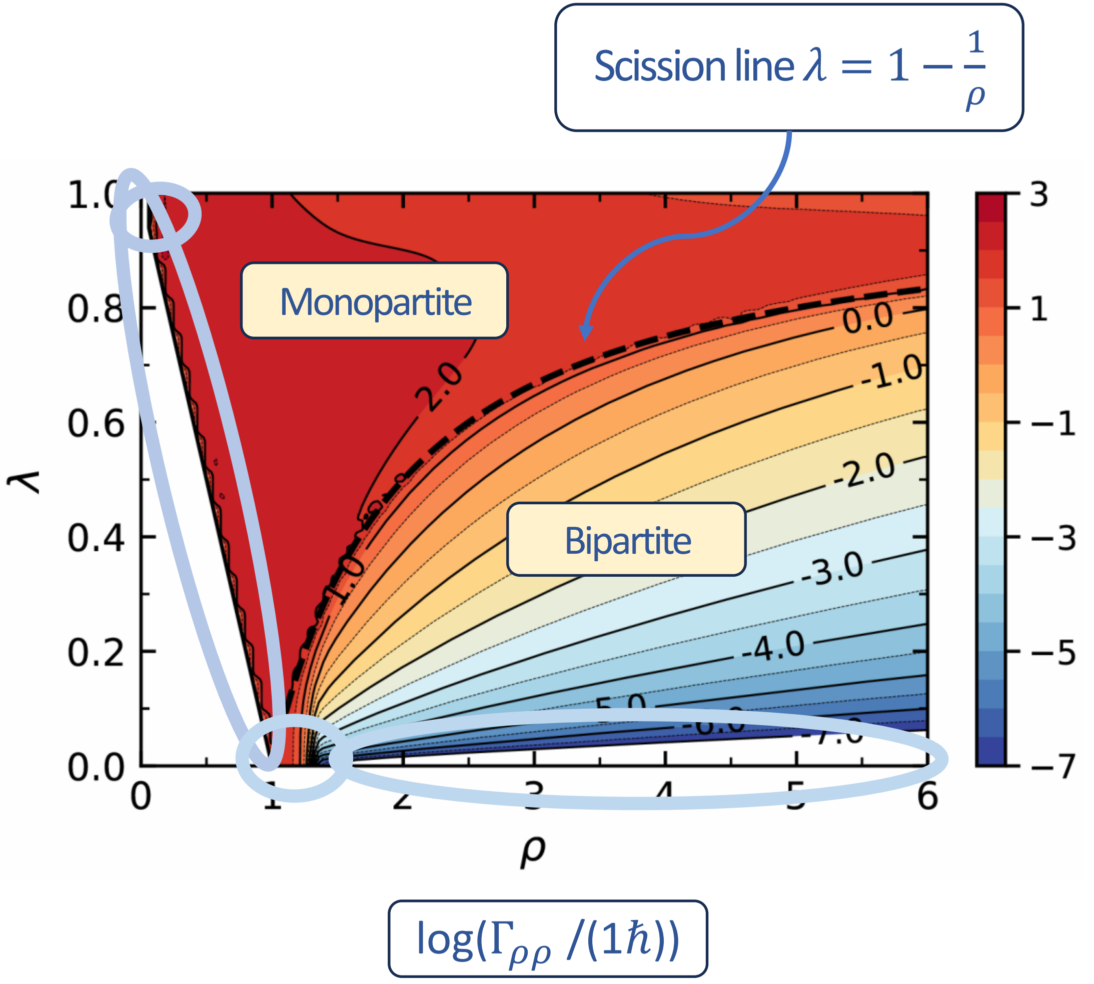
W. Przystupa, K. Pomorski, Nucl. Phys. A 572(1) (1994) 153

- Systems: ^{64}**Ni** + ^{92,96}**Zr** → ^{156}**Er**
- **Minimal shells effects** at the incident energies (50 MeV).
- Calculations with the **asymmetry variable frozen**.
- **Correction of the diffusion tensor** by a factor 6 to reproduce the tails of the spin distributions
- **Possible improvement**:
  - **Full calculation** with asymmetry needed



Physical vs. practical collective variables

- Unlike the multipole moments, the (ρ, λ, σ) variables are **extremely irregular**:
  - **Many borders,**
  - **Small proximity region,**
  - **Regime change.**
- **A correct treatment of numerical precision is needed.**
- **Extrapolation** is needed for the calculations of the physical quantities and their derivatives.
  The regions of extrapolation should **avoid the borders.**
- The process of fusion itself is not fully tractable numerically.



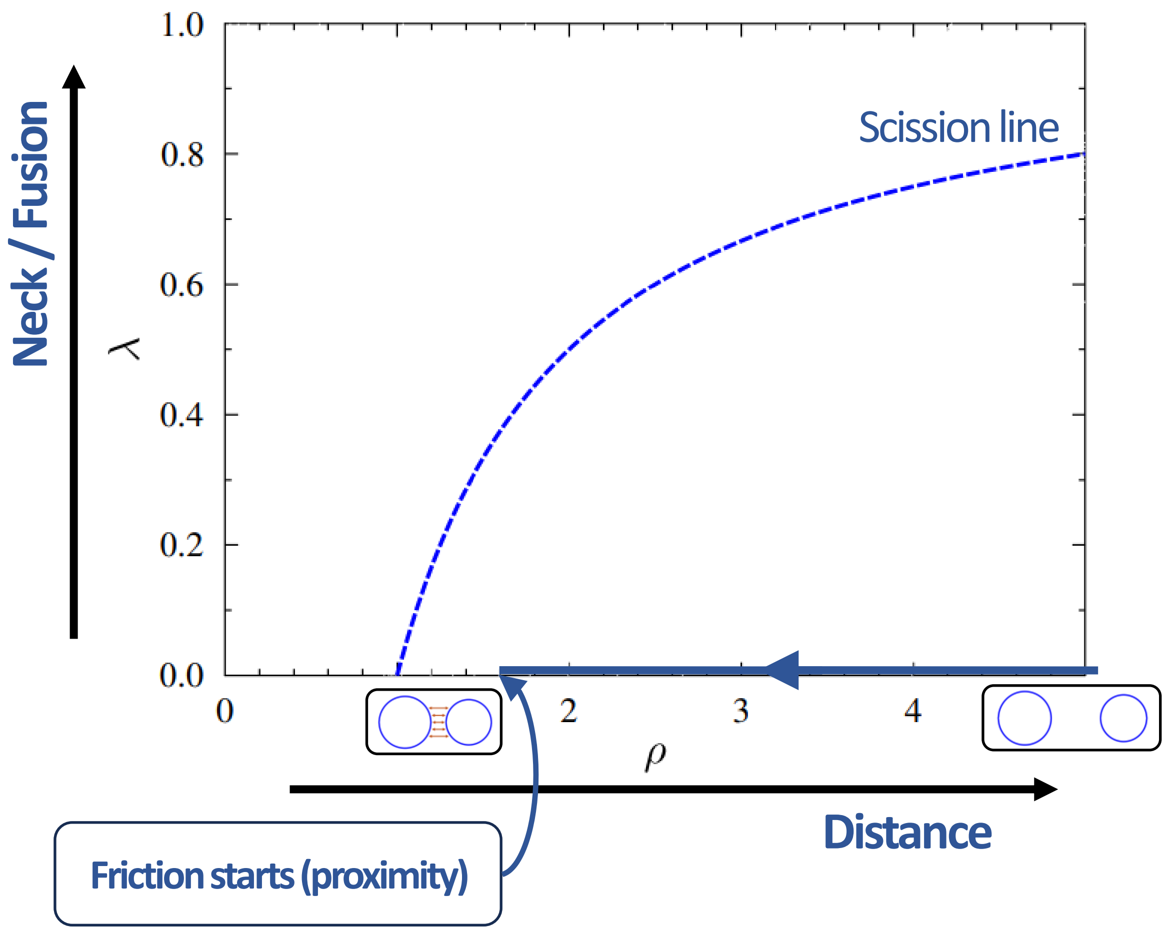
The fusion process

The three main stages of the collision:

1. **A first violent deceleration** during which:
   - The **system loses most of its kinetic energy**
   - There is **almost no deformation of the nuclei**

   $(\dot{\lambda} = (\mathcal{M}_{\rho\lambda})^{-1} p_\rho + (\mathcal{M}_{\lambda\lambda})^{-1} p_\lambda = -\infty + \infty)$

   - **Unstable balance close to the lambda border**



The fusion process

The three main stages of the collision:

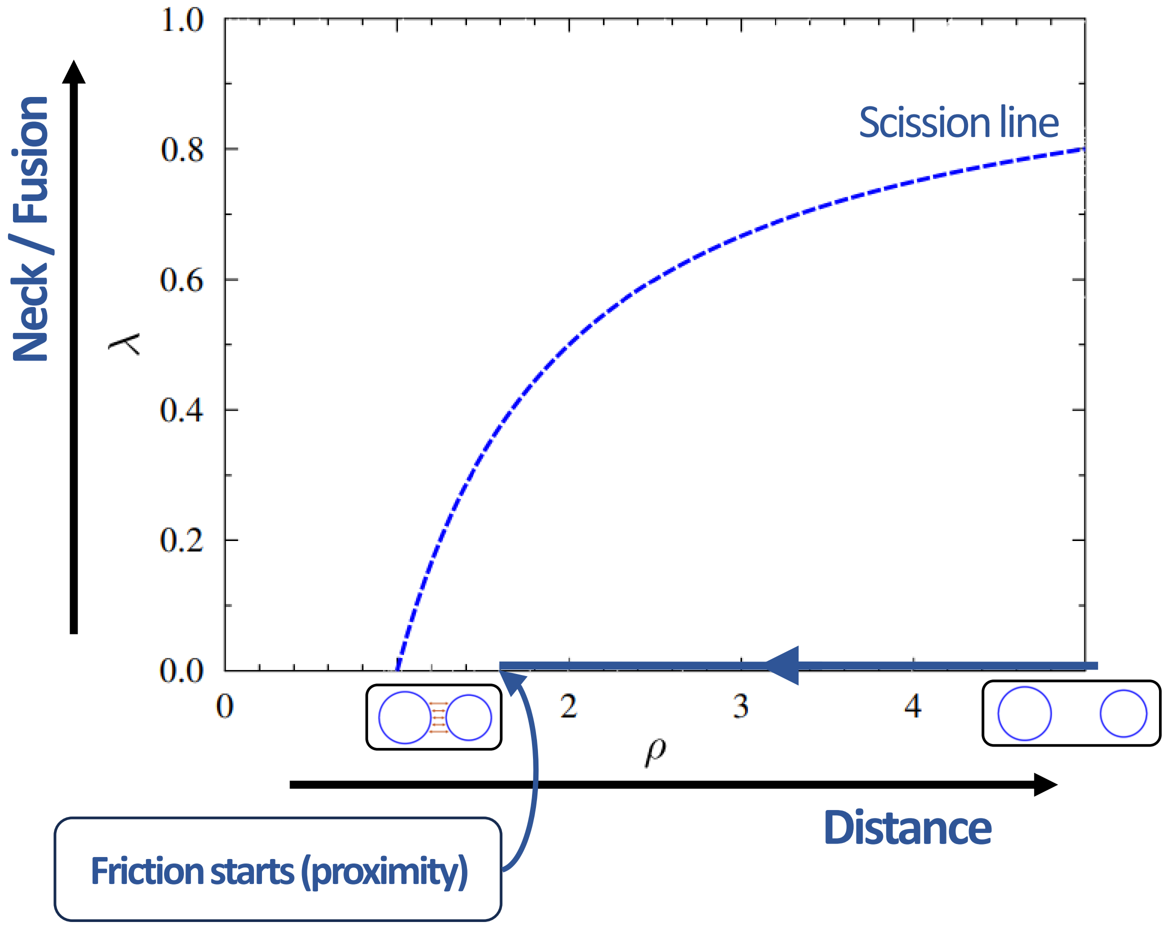
1. **A first violent deceleration** during which:
   - The **system loses most of its kinetic energy**
   - There is **almost no deformation of the nuclei**

   $$(\dot{\lambda} = (\mathcal{M}_{\rho\lambda})^{-1} p_\rho + (\mathcal{M}_{\lambda\lambda})^{-1} p_\lambda = -\infty + \infty)$$

   - **Unstable balance close to the lambda border**

   - **Physical interpretation: (Extra)-deformation can only occur when the fragments interact with each other**

   - **Treated exactly** (conservative forces).

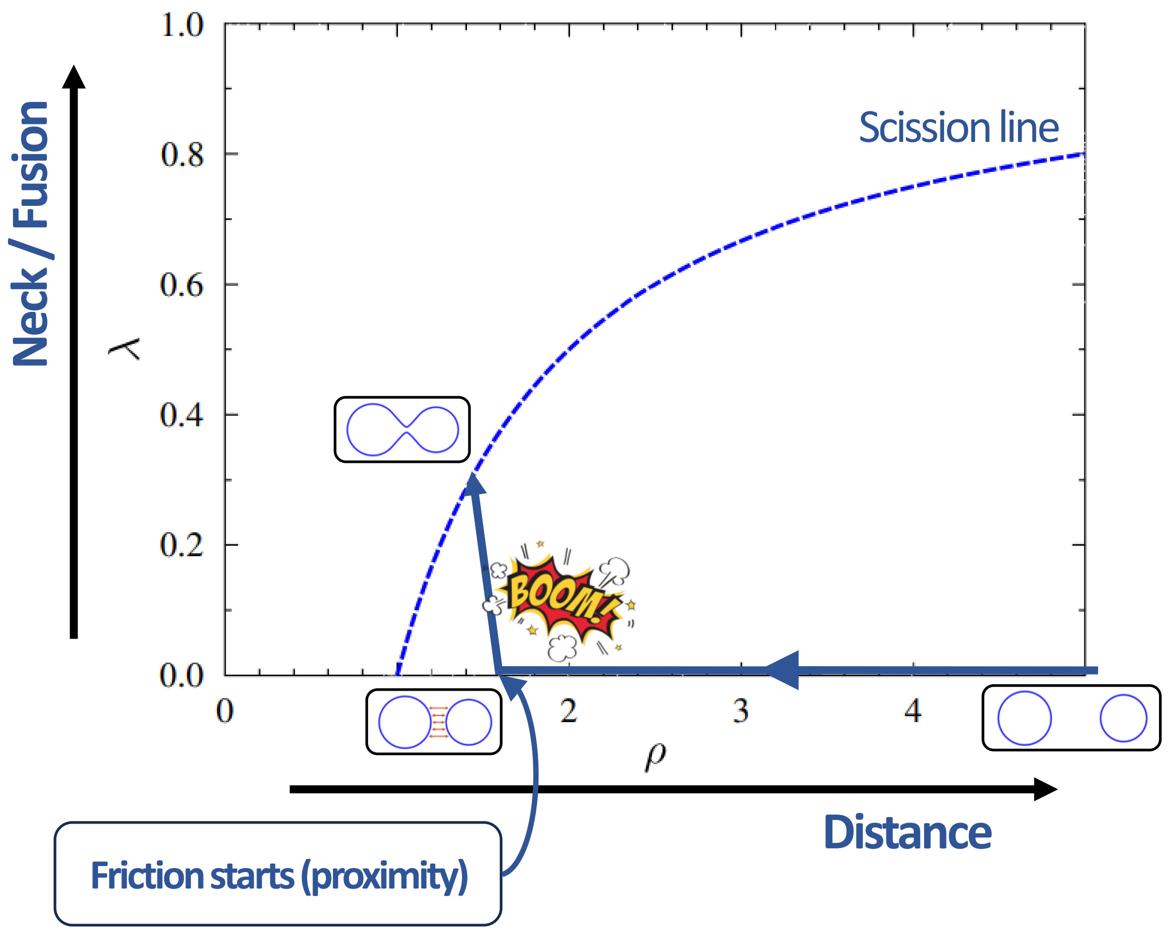


The fusion process

2. The **"Kiss of death"** when friction starts

- **A little sudden change in** p_ρ → **infinite push to the scission line** $(\dot{\lambda} = (\mathcal{M}_{\rho\lambda})^{-1} p_\rho + (\mathcal{M}_{\lambda\lambda})^{-1} p_\lambda = -\infty + \infty)$

- **Deformation starts and remains.**



The fusion process

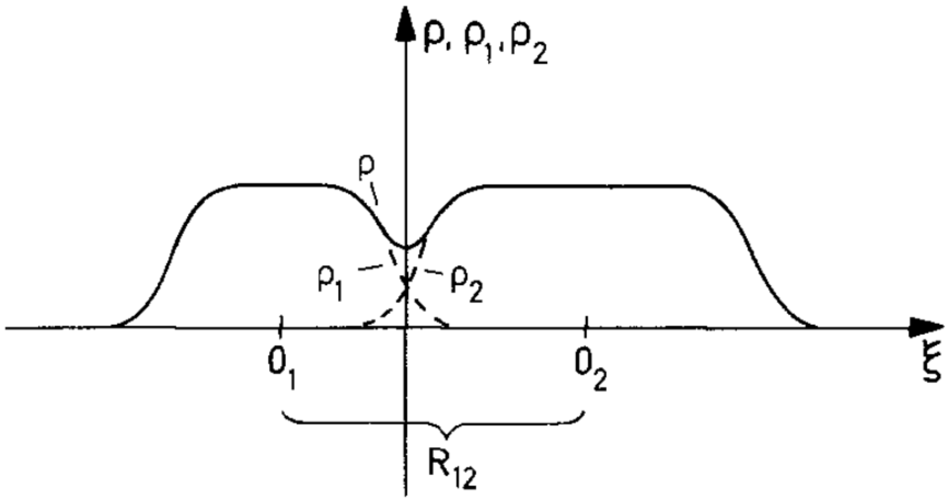
2. The **"Kiss of death"** when friction starts

   - **A little sudden change in** p_ρ **→ infinite push to the scission line** $\left(\dot{\lambda} = (\mathcal{M}_{\rho\lambda})^{-1} p_\rho + (\mathcal{M}_{\lambda\lambda})^{-1} p_\lambda = -\infty + \infty\right)$

   - **Deformation starts and remains.**

   - **Inherent instability of non-saturated nucleonic densities** (**Sudden approximation** in HF when the nuclear tails touch)

   - **This step is <u>NOT</u> treated numerically**: We start the calculation from the touching point

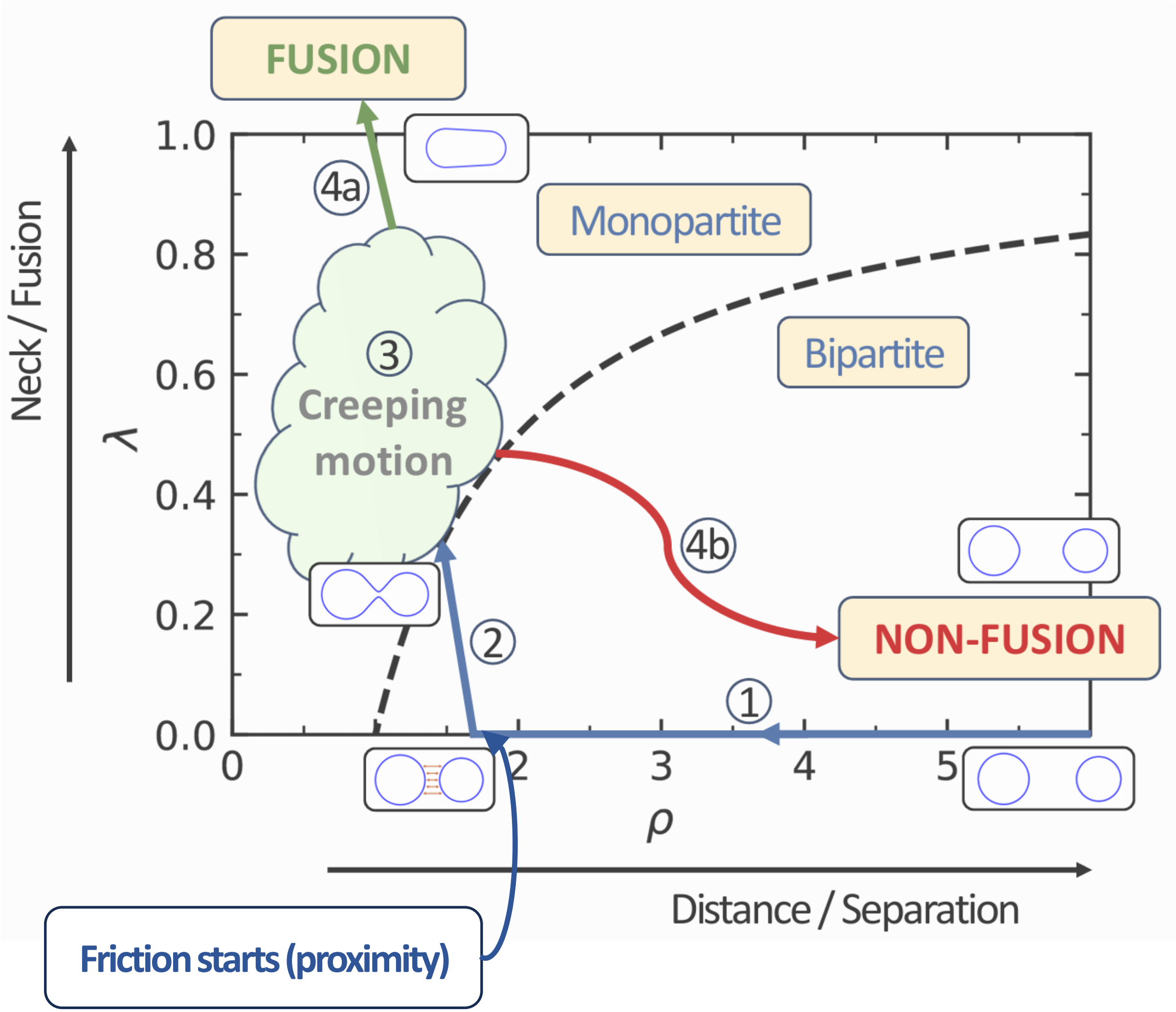


"Sudden approximation" – K. Pomorski, K. Dietrich Z. Phys. A, 295 (1980) 335

The fusion process

The three main stages of the collision:

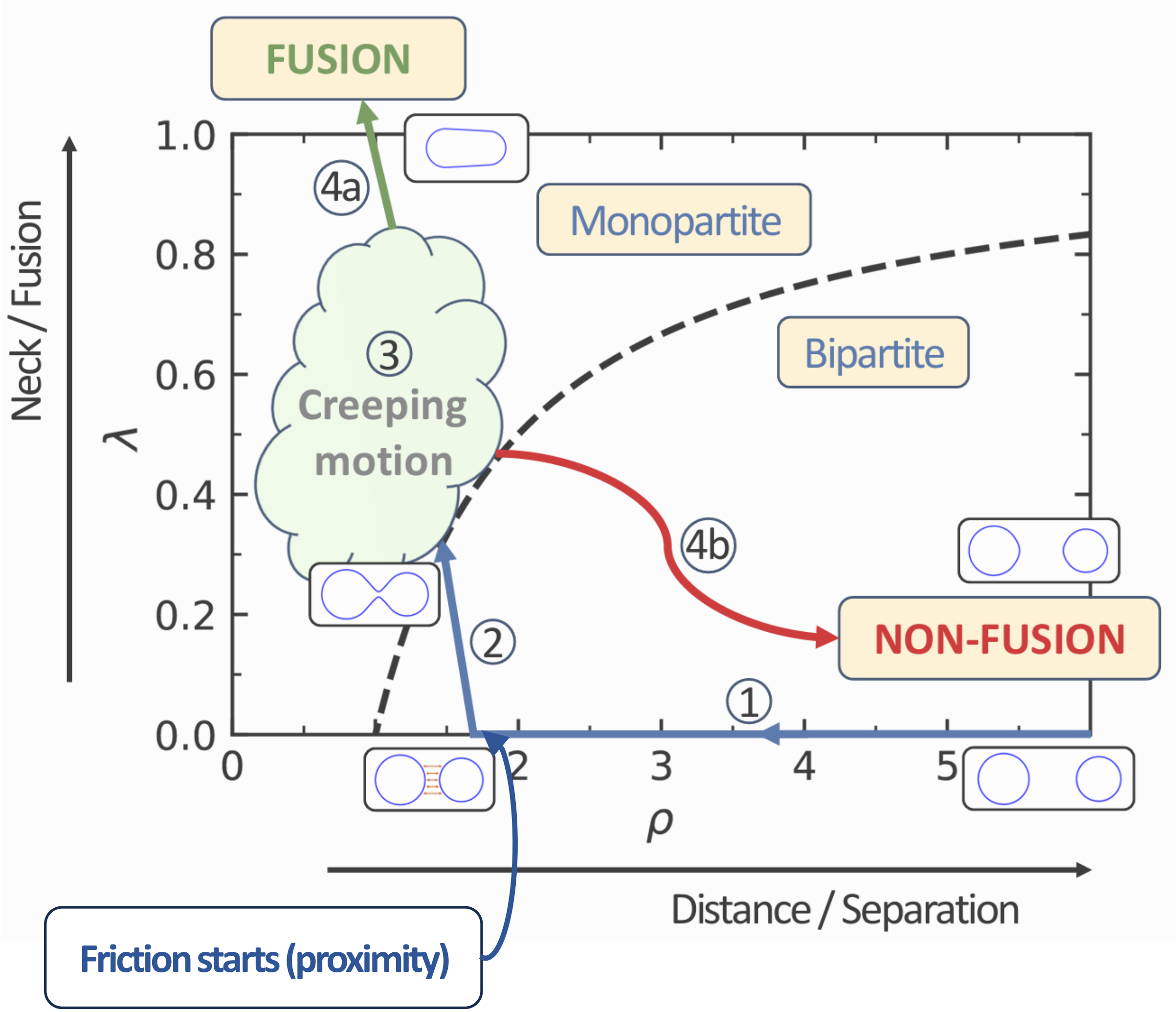
3. A **long creeping motion**
   - which leads to fusion or separation
   - **Solved numerically**



Defining fusing and non-fusing events

- **Fusing conditions**:
  - $\lambda = 1$ (half of the spheres are mixed)
  - $\rho(1-\lambda) = \Delta^2$ (window angle fully open)
  - $\rho = 0.5$

- **Non-fusing conditions**:
  - $\lambda \to \lambda_{min} = 10^{-2}$
  - $\rho \to \rho_{max} = 3$
  - No fusion after $N_{max} = 500{,}000$ steps.



The observables

- The resolution of the Langevin equations generates **a distribution of trajectories due to the fluctuation force.**
- We use **500,000 - 1,000,000 trajectories.**
- **Asymmetry is free to change**.
- Calculations performed on the **CiŚ cluster** (Świerk/Warsaw).

- The **spin distribution** is calculated as a Monte-Carlo integral on a given bin $i \equiv \ell_i$:

$$\sigma_\ell = \left(\frac{d\sigma_{fus}}{d\ell}\right)_{\ell_i} = \frac{2\pi}{k^2}\ell_i^2 \frac{N_i^{fus}}{N_i^{tot}}$$

where $\ell_{init} = \ell_{max}\sqrt{x}, x$ a random number in [0,1] (for easy derived formulas).

- From the spin distribution, one can calculate:
  - The **total cross section / probability for the formation of the compound nucleus**
  - $\langle \ell \rangle , \langle \ell^2 \rangle$
  - **Excitation functions.**

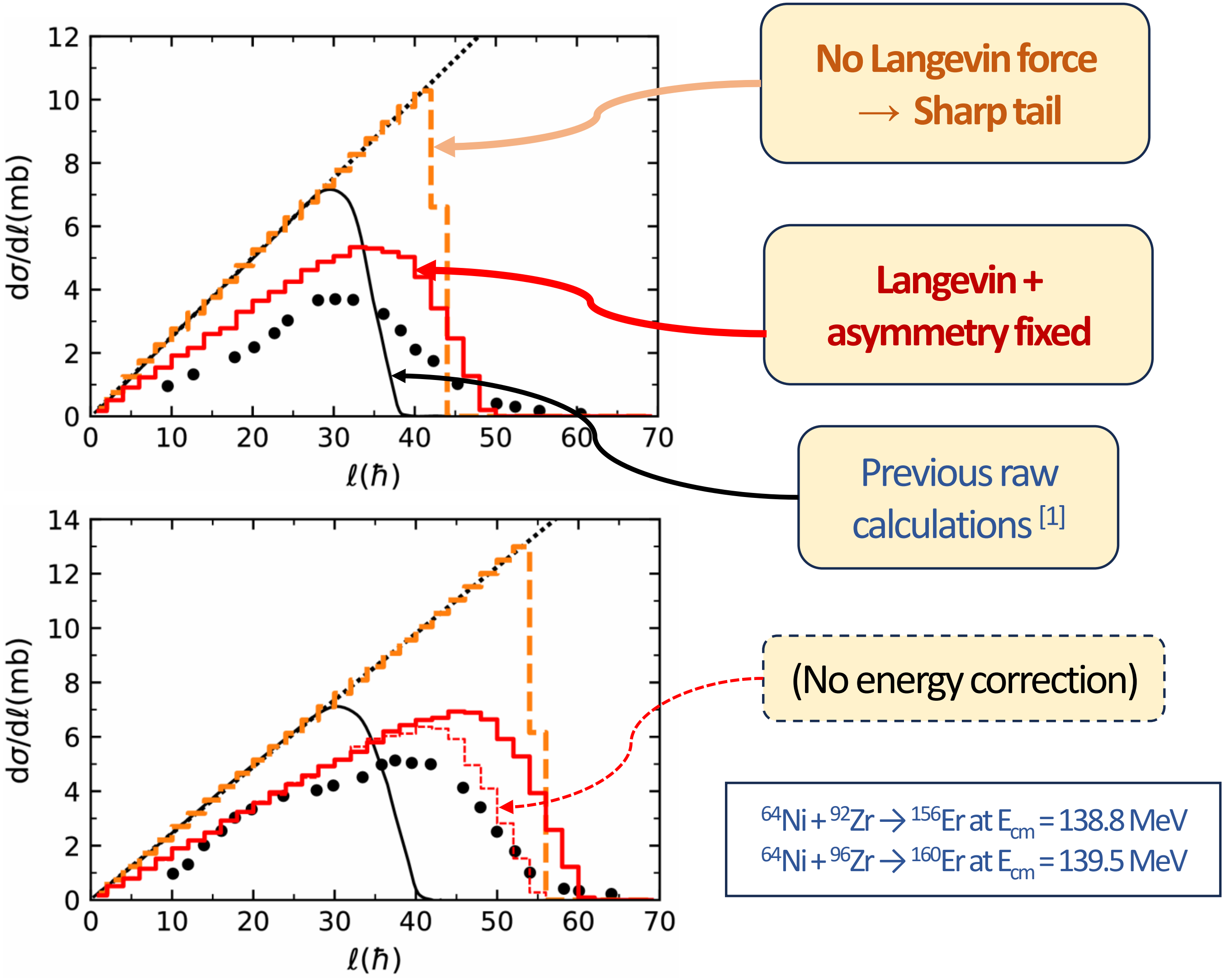
^{64}Ni + ^{92,96}Zr ⟶ ^{156,160}Er – Asymmetry fixed

- ^{64}Ni + ^{92}Zr: $Q_{fus,calc} = Q_{fus,exp}$ ⟶ no correction needed
- ^{64}Ni + ^{96}Zr: Difference of 3.5 MeV ⟶ **correction needed**
  Effect of deformation?

- **Spin distributions are more natural with the Langevin force.**
- They **drop at the correct angular momentum**
  ⟶ Relevant for a correct description of fission.

- The experimental data come from Refs. [2,3]

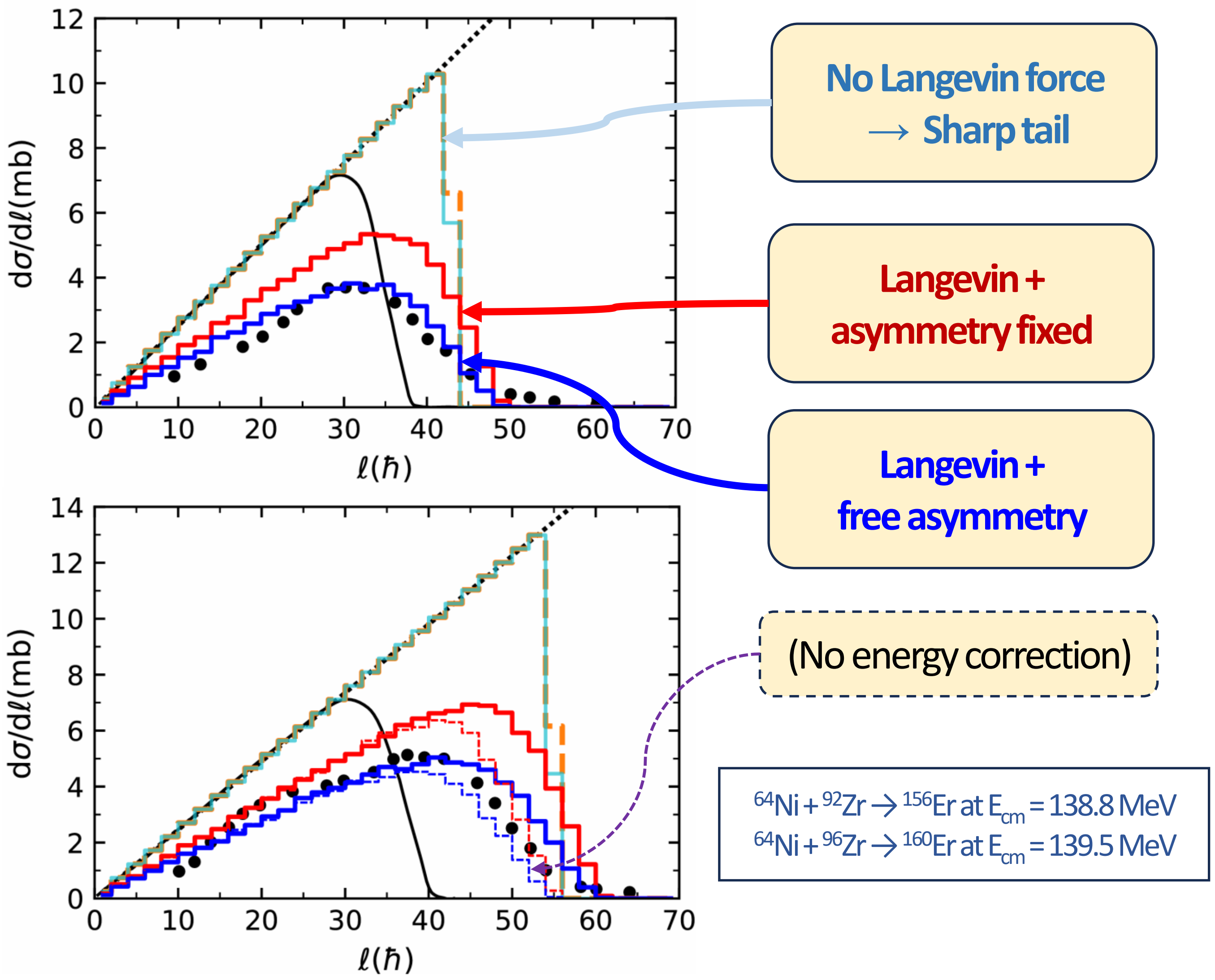
[1] W. Przystupa, K. Pomorski, Nucl. Phys. A 572(1) (1994) 153
[2] W. Kuhn *et al.*, Phy. Rev. Lett. 62 (1989) 1103
[3] A. M. Stefanini *et al.*, Phys. Lett. B 252 (1990) 43



^{64}Ni + ^{92,96}Zr $\longrightarrow$ ^{156,160}Er – Effect of the Asymmetry

- The release of the **asymmetry decreases the spin distributions** (non-asymmetrical case)
- **Great agreement to the experimental data[2,3] .**
- In the ^{64}Ni + ^{96}Zr case, little discreprancies in the spin distributions, despite the energy correction
- **The total cross section (160 mb) is well reproduced.**

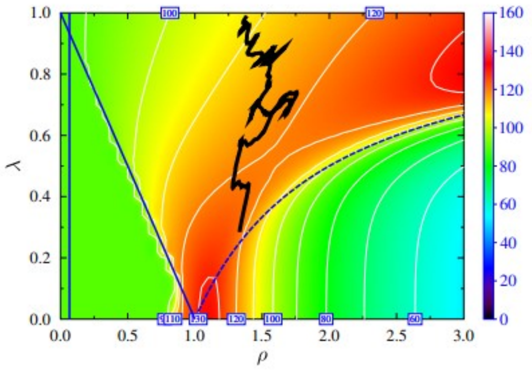
[1] W. Przystupa, K. Pomorski, Nucl. Phys. A 572(1) (1994) 153
[2] W. Kuhn *et al.*, Phy. Rev. Lett. 62 (1989) 1103
[3] A. M. Stefanini *et al.*, Phys. Lett. B 252 (1990) 43

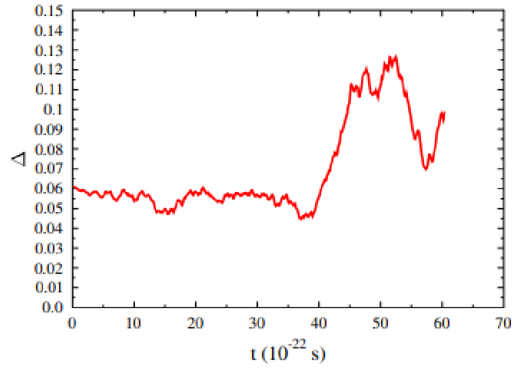


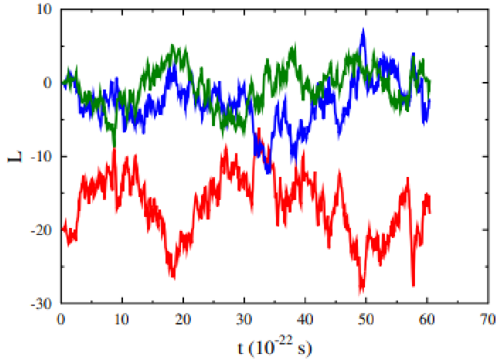
A deep understanding of the fusion process (Preliminary examples)

Paths | Asymmetry vs. time | Angular momenta

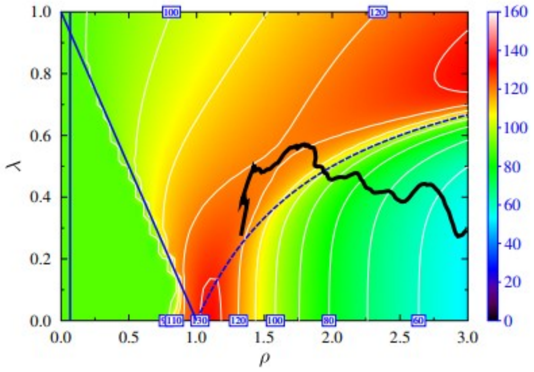
- $\ell = 20\hbar$,
  Fusion case:

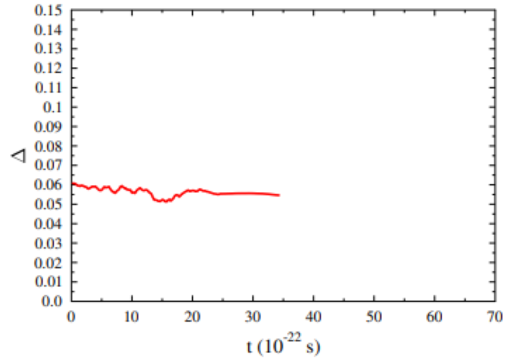


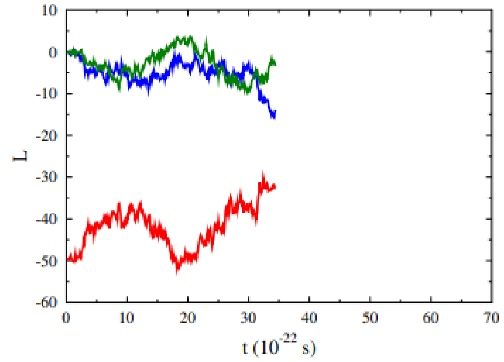




- $\ell = 50\hbar$,
  No-fusion case:







- And various other observables: **diffusion tensor**, the **number of rotations the system udergoes before fusion** etc.

Summary and Perspectives

- We have derived a fully **6-dimensional dissipative dynamics Langevin**-based formalism to describe the **unrestricted motion of the systems** in terms of **elongation**, **neck** and **asymmetry** variables.

- Thanks to a **correct treatment of the different stages of fusion**, the spin distributions are now **in great agreement with experimental data**.
- The Langevin formalism allows for a deep understanding of the fusion process: evolution of the asymmetry, angular momentum/rotations of the fragments etc.

- In the future:
  - We will study the effect of the **asymmetry of entrance channel** on the formation of the compound system.
  - We will tackle the **hindrance problem** by comparing the ^{48}**Ca/**^{50}**Ti/**^{54}**Cr +** ^{208}**Pb** systems.

- We are planning to make the following improvements of the formalism:
  - The addition of **shell effects** for a **fully microscopic-macroscopic picture**
  - The testing of different forms of stochastic noises (**color noises**),
  - The incorporation of **neutron emission** throughout the process.

Summary and Perspectives

- We have derived a fully **6-dimensional dissipative dynamics Langevin**-based formalism to describe the **unrestricted motion of the systems** in terms of **elongation**, **neck** and **asymmetry** variables.

- Thanks to a **correct treatment of the different stages of fusion**, the spin distributions are now **in great agreement with experimental data**.
- The Langevin formalism allows for a deep understanding of the fusion process: evolution of the asymmetry, angular momentum/rotations of the fragments etc.

- In the future:
  - We will study the effect of the **asymmetry of entrance channel** on the formation of the compound system.
  - We will tackle the **hindrance problem** by comparing the ^{48}**Ca/**^{50}**Ti/**^{54}**Cr +** ^{208}**Pb** systems.

- We are planning to make the following improvements of the formalism:
  - The addition of **shell effects** for a **fully microscopic-macroscopic picture**
  - The testing of different forms of stochastic noises (**color noises**),
  - The incorporation of **neutron emission** throughout the process.

Thank you for your attention!