Comparative Study of Langevin and Random Walk Models for Nuclear Fission

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Motivation and central question

- Nuclear fission is a dissipative large-amplitude collective motion.
- Fragment mass yields are shaped during the descent from the outer saddle to scission.
- Two stochastic descriptions are compared on the same potential energy surfaces:
  - multidimensional Langevin dynamics,
  - Metropolis random walk / Brownian shape motion.
- Main question: when does the random walk reproduce the overdamped Langevin limit?

Studied systems

Thermal neutron-induced fission of selected actinides:

$^{229}\mathrm{Th}$, $^{231}\mathrm{Pa}$, $^{235}\mathrm{U}$, $^{237}\mathrm{Np}$, $^{239}\mathrm{Pu}$,

$^{241}\mathrm{Am}$, $^{245}\mathrm{Cm}$, $^{249}\mathrm{Cf}$, $^{254}\mathrm{Es}$, $^{255}\mathrm{Fm}$.

Key comparison

Same FoS shape space, same PES input, different stochastic dynamics.

Common theoretical framework

Fourier-over-Spheroid shape space

The collective coordinates are

$$\boldsymbol{q} = \{c, a_3, a_4, \eta\},$$

where

- c — elongation,
- a_3 — mass asymmetry,
- a_4 — neck degree of freedom,
- η — triaxiality.

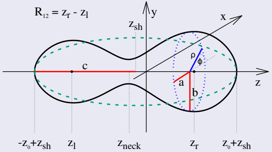
For the dynamics beyond the outer saddle the PES is minimized over η, giving an effective 3D space:

$$\boldsymbol{q} = \{c, a_3, a_4\}.$$

Macro–micro potential

$$V(\boldsymbol{q}, T) = V_{\rm mac}(\boldsymbol{q}) + V_{\rm mic}(\boldsymbol{q}, T).$$

$$V_{\rm mic}(\boldsymbol{q}, T) \approx V_{\rm mic}(\boldsymbol{q}, 0) \left[1 + \exp\left(\frac{T - 1.5}{0.3}\right)\right]^{-1}$$



FoS shapes illustrate the evolution from compact to elongated, necked, and mass-asymmetric configurations near scission.

Fourier-over-Spheroids shape parametrization

Nuclear surface

In the Fourier-over-Spheroids parametrization, the nuclear surface is written in cylindrical coordinates (ρ, φ, z) as

$$\rho^2(z,\varphi) = \frac{R_0^2}{c}\, f\left(\frac{z - z_{\rm sh}}{z_0}\right) \frac{1-\eta^2}{1+\eta^2+2\eta\cos(2\varphi)}.$$

Geometrical meaning

- R_0: radius of the spherical nucleus.
- $z_0 = cR_0$: half-length of the system.
- $z_{\rm sh}$: center-of-mass shift.
- η: triaxiality parameter.

Axial profile

For the four-dimensional deformation space:

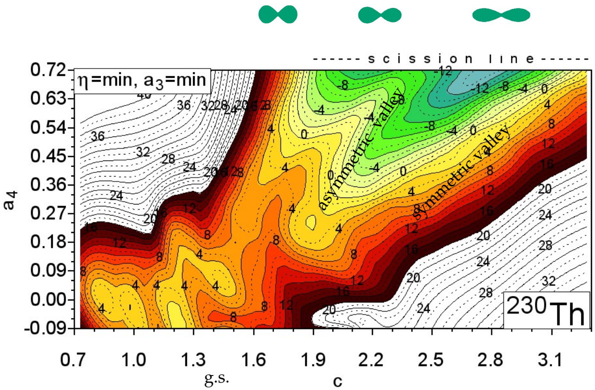
$$z_{\rm sh} = -\frac{3}{4\pi} z_0 a_3,$$

$$f(u) = 1 - u^2 - a_2 \cos\left(\frac{\pi u}{2}\right) - a_3 \sin(\pi u) - a_4 \cos\left(\frac{3\pi u}{2}\right),$$

with

$$u = \frac{z - z_{\rm sh}}{z_0}.$$

Potential energy surface and fission valleys



- Example: ^{230}Th PES at $T = 0$ MeV.
- Projection onto the (c, a_4) plane after minimization over a_3 and η.
- Characteristic actinide structure:
    - ground-state minimum,
    - first barrier,
    - second minimum,
    - outer saddle,
    - asymmetric and symmetric valleys.
- Low-energy fission starts near the outer saddle.

Langevin dynamics

Coordinates and momenta

$$\frac{dq_i}{dt} = \sum_j [m^{-1}(\boldsymbol{q})]_{ij} p_j .$$

$$\frac{dp_i}{dt} = -\frac{\partial V(\boldsymbol{q},T)}{\partial q_i} - \frac{1}{2}\sum_{jk} \frac{\partial [m^{-1}(\boldsymbol{q})]_{jk}}{\partial q_i} p_j p_k - \sum_{jk} \gamma_{ij}(\boldsymbol{q},T)[m^{-1}(\boldsymbol{q})]_{jk} p_k + \sum_j g_{ij}(\boldsymbol{q})\Gamma_j(t).$$

- Inertia: Werner–Wheeler approximation.
- Friction: Wall formula with phenomenological temperature dependence.
- Noise: Gaussian white noise.
- Scission condition:

$$R_{\rm neck} \approx 1.2\ \mathrm{fm} \quad \Longleftrightarrow \quad a_4 \approx 0.72.$$

Physics content

Langevin trajectories retain finite inertia and memory even in a strongly damped regime.

Fluctuation–dissipation relation and effective temperature

Intrinsic excitation

$$E_{\rm int} = E_{\rm tot} - \frac{1}{2}\sum_{ij}[m^{-1}(\boldsymbol{q})]_{ij}p_i p_j - V(\boldsymbol{q}, T=0),$$

$$E_{\rm int} = a(\boldsymbol{q})T^2.$$

Noise strength

$$\sum_k g_{ik}(\boldsymbol{q})g_{jk}(\boldsymbol{q}) = \gamma_{ij}(\boldsymbol{q}, T)T^*.$$

Quantum-corrected temperature

$$T^* = \frac{E_0}{\tanh(E_0/T)}, \qquad E_0 \approx 1.5 \text{ MeV}.$$

- $T \to 0$: $T^* \to E_0$.
- $T \to \infty$: $T^* \to T$.
- Mimics zero-point fluctuations in a Markovian Langevin framework.

Friction: phenomenological temperature dependence

Adopted friction tensor

$$\gamma_{ij}(\boldsymbol{q}, T) = \frac{\left(\frac{2}{3} - \varepsilon\right) \gamma_{ij}^{\mathrm{wall}}(\boldsymbol{q})}{1 + \exp\left[(1.3 - T)/0.2\right]} + \varepsilon \gamma_{ij}^{\mathrm{wall}}(\boldsymbol{q}), \qquad \varepsilon = 0.01.$$

- Low T: pairing suppresses effective dissipation.
- Higher T: friction approaches a fraction of the Wall limit.
- Strong-friction reference case:

$$\gamma_{ij} = \frac{2}{3} \gamma_{ij}^{\mathrm{wall}}.$$

Interpretation

The default calculation represents moderately damped saddle-to-scission motion, while the strong-friction case probes the overdamped regime.

Metropolis random walk model

Overdamped limit

In the strong-friction limit, momenta cease to be independent dynamical variables and the evolution becomes diffusive in coordinate space.

$$E_{\rm int}(\boldsymbol{q}) = E_{\rm tot} - V(\boldsymbol{q}, T).$$

$$\rho(E_{\rm int}) \propto \exp\left(2\sqrt{a_0 E_{\rm int}}\right), \qquad a_0 = A/8.5\ \mathrm{MeV}^{-1}.$$

Metropolis step

A neighboring point $\boldsymbol{q}_j$ is accepted with probability

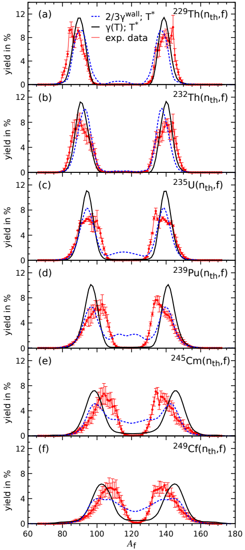
$$P_{i\to j} = \min\left[1, \frac{\rho(E_{\rm int}(\boldsymbol{q}_j))}{\rho(E_{\rm int}(\boldsymbol{q}_i))}\right].$$

- 26 nearest neighbors on the 3D grid.
- Uniform grid spacing:

$$\Delta c = \Delta a_3 = \Delta a_4 = 0.01.$$

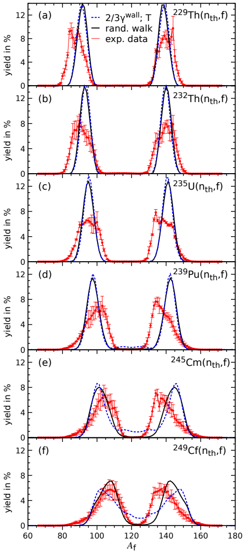
- Scission again at $a_4 \approx 0.72$.

Langevin results: mass-yield systematics



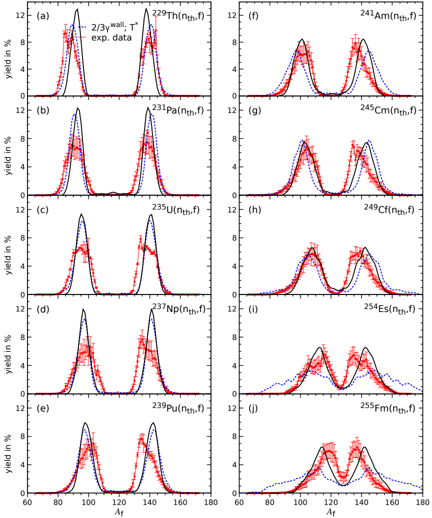
- Black curves: phenomenological temperature-dependent friction with T^*.
- Blue curves: high-friction limit, $\gamma = \frac{2}{3}\gamma^{\rm wall}$, with T^*.
- Experimental symbols: evaluated post-neutron data.
- Default Langevin reproduces the dominant asymmetric peaks.
- High friction plus T^* enhances diffusion and tends to overpopulate symmetric fission.

Random walk versus overdamped Langevin



- Black curves: Metropolis random walk.
- Blue curves: Langevin with $\gamma = \frac{2}{3}\gamma^{\mathrm{wall}}$ and classical T instead of T^*.
- Excellent agreement for lighter actinides.
- Deviations grow for Cm and Cf.
- Langevin may retain residual inertial effects absent in the purely configurational random walk.

Weak damping of shell effects with temperature



Physical picture

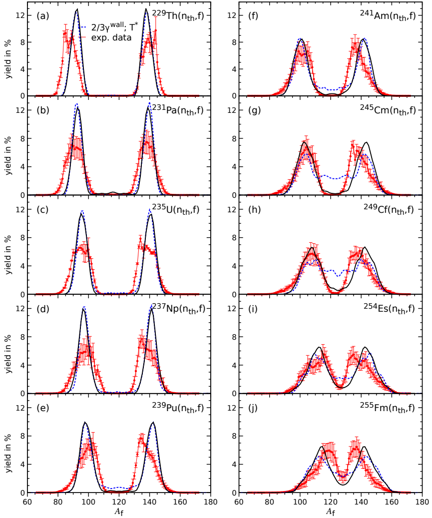
In this case the microscopic shell corrections decrease only slowly with increasing temperature. As a consequence, shell effects remain important over a broader range of excitation energy.

Interpretation

Weak damping of shell effects preserves the structure of the potential-energy surface, including the valleys and ridges that guide the fission path.

- Shell-induced minima and barriers remain visible.
- The asymmetric fission valleys stay well pronounced.
- The system remains more sensitive to microscopic structure effects.
- Fragment yields retain a stronger shell-driven character.

Strong damping of shell effects with temperature



Physical picture

Here the microscopic shell corrections are damped much more rapidly with increasing temperature. The shell structure is washed out earlier, and the energy landscape becomes smoother.

Interpretation

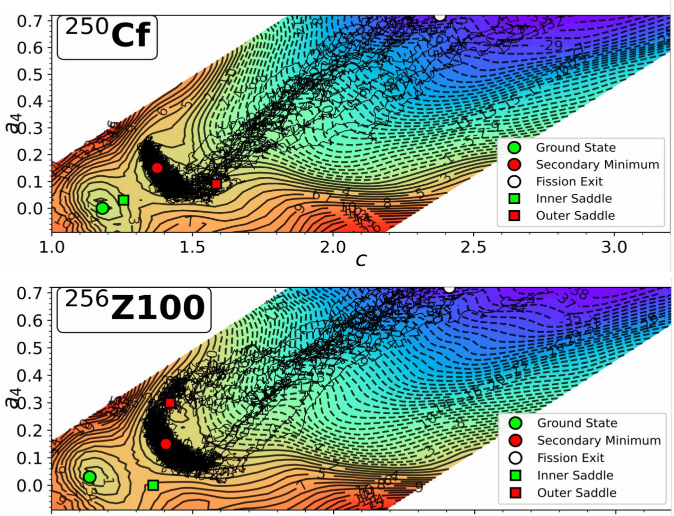
Strong damping reduces the role of shell effects in shaping the fission path, so the dynamics becomes more controlled by the macroscopic component of the potential.

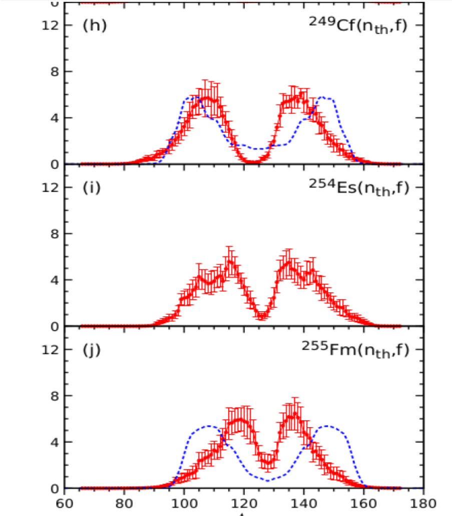
- Shell-induced structures become less pronounced.
- The distinction between competing valleys is reduced.
- The system evolves on a smoother PES.
- Fragment yields are less constrained by microscopic shell structure.

Trajectories on the PES and heavy-actinide mass yields

Left: selected Langevin trajectories on the PES, started from the second minimum after neutron capture. Right: corresponding mass-yield systematics for heavier systems, where the symmetric component becomes more sensitive to shell damping and diffusion.

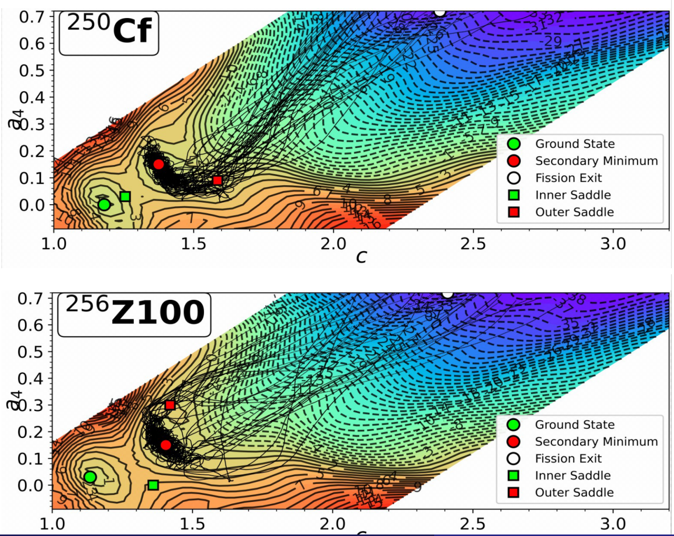
$\gamma_{ij} = \frac{2}{3}\gamma_{ij}^{\rm wall}$, T instead of T^*.

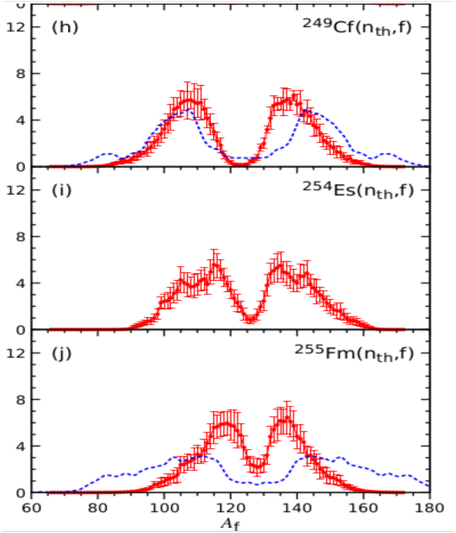




Trajectories on the PES and heavy-actinide mass yields

Left: selected quantum Langevin trajectories on the PES, started from the second minimum after neutron capture.
Right: corresponding mass-yield systematics for the same conditions. $\gamma_{ij} = \gamma_{ij}(T)$, T^* in the fluctuation–dissipation relation.

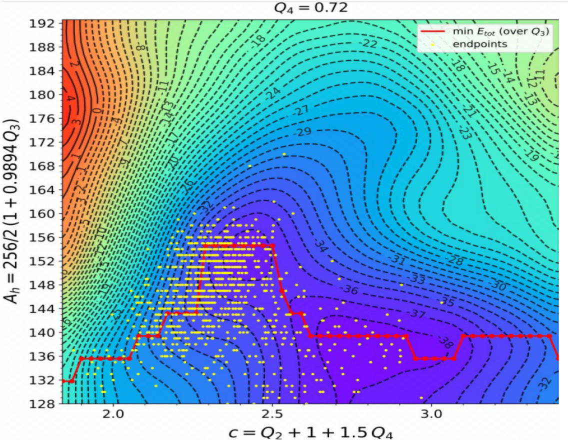




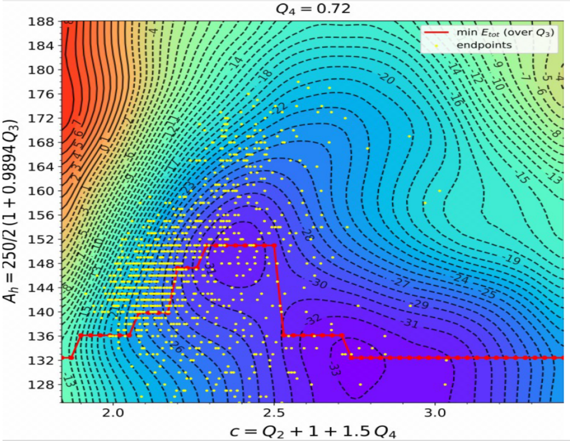
Classical vs quantum Langevin at scission

The maps are shown for the scission condition $Q_4 = 0.72$.Yellow dots denote trajectory endpoints, while the red curve shows the minimum of the total energy with respect to Q_3.

Ordinary (classical) Langevin



Quantum Langevin



Langevin vs. Metropolis random walk

Scope of the comparison

- Both approaches were compared within the same Fourier-over-Spheroid deformation space and on the same macroscopic–microscopic PES.
- The purpose was to test to what extent a purely configurational, overdamped Metropolis walk can reproduce the dynamical Langevin evolution.

Main findings

- For lighter actinides, the agreement is very good: in the high-friction regime the Metropolis walk reproduces the overdamped Langevin limit.
- The agreement gradually worsens for heavier nuclei, especially Cm and Cf.
- In these systems, Langevin trajectories retain residual inertia and can still access competing valleys, including the symmetric one.
- The quantum-corrected temperature T^* enhances diffusion and may strengthen the symmetric fission component at intermediate excitation energies.

Physical origin of the discrepancies

What controls the yields?

- The final mass split is governed primarily by the topology of the potential-energy surface.
- The decisive ingredients are the asymmetric valleys, inter-valley ridges, and the structure of the scission region.
- Weak damping preserves shell-driven guidance in the PES, while strong damping smooths the dynamics and reduces the microscopic selectivity of the trajectories.

Why does the agreement break down for heavier nuclei?

- In very heavy systems the present dissipation may become too weak, pushing the Langevin motion toward a partially ballistic regime.
- Then the formal difference between the two methods becomes essential: the random walk remains overdamped and configurational, whereas Langevin motion retains memory of collective momentum.
- This may lead to broader and less localized yields, as seen in preliminary fermium calculations.

Model limitations and outlook

Current limitations

- The collective space is restricted to $\{c, a_3, a_4\}$ on an η-minimized PES; missing coordinates may open additional paths toward scission.
- The present scission criterion is purely geometrical ($a_4 \simeq 0.72$) and may terminate trajectories too early in very heavy nuclei.
- The dissipation model is based on wall friction with phenomenological temperature dependence and does not explicitly include window friction associated with nucleon exchange through the neck.

Outlook

- A quantitative description of fermium and heavier systems likely requires an extended collective space, a refined scission treatment, and an improved dissipation prescription.
- A promising strategy is a hybrid approach combining the efficiency of random-walk sampling with the dynamical realism of full Langevin evolution.

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Dissipation in heavy-ion and fission dynamics

Physical motivation

Dissipative phenomena in nuclear shape evolution resemble generalized Brownian motion: a few macroscopic collective coordinates interact with many microscopic intrinsic degrees of freedom.

Collective subsystem

The slow variables describe large-scale nuclear motion:

$$\mathbf{q} = \{q_1, \ldots, q_n\}, \qquad \mathbf{p} = \{p_1, \ldots, p_n\}.$$

Examples:

- elongation,
- mass asymmetry,
- neck formation,
- relative distance in heavy-ion collisions.

Intrinsic heat bath

The fast microscopic degrees of freedom are associated with nucleonic motion. They absorb collective kinetic energy and generate:

- friction,
- fluctuations,
- irreversible heating,
- conversion of ordered motion into intrinsic excitation.

In fission, dissipation controls how the system descends from saddle to scission and how strongly trajectories diffuse between competing valleys.

General Langevin picture of nuclear dissipation

Macroscopic variables and stochastic dynamics

A set of collective coordinates and momenta evolves under conservative, dissipative, and fluctuating forces:

$$\dot{p}_i = K_i(\mathbf{p}, \mathbf{q}) + X_i(t), \qquad i = 1, \ldots, n,$$

$$\dot{q}_i = \sum_k M^{-1}_{ik}(\mathbf{q}) p_k .$$

Conservative force

If the macroscopic motion is described by a Hamiltonian

$$H(\mathbf{p}, \mathbf{q}) = T(\mathbf{p}, \mathbf{q}) + V(\mathbf{q}),$$

then

$$K_i = -\frac{\partial H}{\partial q_i} = -\frac{\partial T}{\partial q_i} - \frac{\partial V}{\partial q_i}.$$

The potential term drives the system along the PES.

Kinetic energy

The collective kinetic energy is determined by the inverse mass tensor:

$$T(\mathbf{p}, \mathbf{q}) = \frac{1}{2} \sum_{ik} p_i M^{-1}_{ik}(\mathbf{q}) p_k .$$

The coordinate dependence of M_{ik} produces additional inertia-gradient forces.

The Langevin equation provides the bridge between deterministic collective motion and stochastic microscopic fluctuations.

One-body dissipation: physical assumptions

Macroscopic viewpoint

The number of participating nucleons is large, so individual particle degrees of freedom do not need to be followed explicitly. The dynamics is projected onto a few collective variables.

Low-temperature regime

At low excitation energy the nuclear temperature is small compared with the Fermi energy. Most nucleons occupy a nearly degenerate Fermi sea.

Leptodermous nucleus

The nucleus has a thin surface:

- surface thickness is small compared with nuclear size,
- saturation and short-range nuclear forces justify a sharp-surface collective description.

Long mean free path

Because of Pauli blocking, two-body nucleon–nucleon collisions are suppressed. The mean free path becomes long, and nucleons behave like a Knudsen gas moving inside a time-dependent nuclear surface.

In this regime, dissipation is dominated by the interaction of nucleons with the moving nuclear surface rather than by ordinary viscous flow.

Wall formula: dissipation from a moving surface

Physical idea

The nuclear surface acts as a moving wall. Nucleons collide with it and exchange momentum with the collective degrees of freedom. This converts collective kinetic energy into intrinsic excitation.

Friction tensor

For axially symmetric shapes, the one-body wall friction tensor can be written as

$$\gamma_{ij}^{\rm wall}(\mathbf{q}) = \frac{1}{2}\pi\rho_m\bar{v}\int_{z_{\rm min}}^{z_{\rm max}} dz\, \frac{\partial\rho_s^2/\partial q_i\,\partial\rho_s^2/\partial q_j}{\left[\rho_s^2 + \frac{1}{4}\left(\frac{\partial\rho_s^2}{\partial z}\right)^2\right]^{1/2}}.$$

Meaning of the ingredients

- ρ_m: nuclear matter density,
- $\bar{v}$: average nucleon speed,
- $\rho_s(z)$: nuclear surface profile,
- q_i, q_j: collective deformation coordinates.

Interpretation

Large surface velocities and strong shape changes increase the coupling between collective motion and intrinsic nucleonic motion.

From friction to fluctuations

Fluctuation–dissipation balance

The same coupling that damps collective motion also generates stochastic fluctuations. In the Langevin framework, both are linked through

$$\sum_k g_{ik}(\mathbf{q}) g_{jk}(\mathbf{q}) = \gamma_{ij}(\mathbf{q}, T) T^* .$$

Dissipative part

Friction removes ordered collective kinetic energy:

$$-\sum_{jk} \gamma_{ij}(\mathbf{q}, T)[m^{-1}(\mathbf{q})]_{jk} p_k .$$

It tends to slow down the collective motion.

Fluctuating part

Random forces re-inject energy into collective degrees of freedom:

$$\sum_j g_{ij}(\mathbf{q}) \Gamma_j(t).$$

They allow trajectories to explore neighboring valleys and occasionally cross inter-valley ridges.

Stronger friction usually implies stronger noise; therefore highly damped motion can become more diffusive on the PES.

Why dissipation matters for fission yields

Weak or moderate damping

- PES topology dominates the descent to scission.
- Trajectories tend to remain in the initially selected valley.
- Asymmetric fission valleys are followed more deterministically.
- Symmetric yield remains suppressed at low excitation energies.

Strong damping

- Noise amplitude increases through fluctuation–dissipation.
- Diffusion across the PES becomes stronger.
- Inter-valley crossing is enhanced.
- Symmetric components may be overpopulated.

Connection with the present work

The comparison between Langevin dynamics and Metropolis random walk tests how far the fission dynamics approaches the overdamped limit and where residual inertia and finite-memory effects remain important.

One-body dissipation: irreversible energy flow

Recoverable vs. unrecoverable energy

Dissipation means an irreversible transformation of accessible collective energy into intrinsic excitation. In a collective model:

- kinetic and potential energies in collective coordinates are recoverable,
- intrinsic excitation energy is only partly recoverable,
- the interaction between collective and intrinsic degrees of freedom produces a flow of energy into the microscopic system.

Measure of irreversibility

The increase of entropy measures the loss of information about the detailed microscopic distribution. Even if total energy is conserved, collective motion can be damped because information is transferred into intrinsic degrees of freedom.

In fission, this is the microscopic origin of the damping of the collective descent from saddle to scission.

What does "one-body" dissipation mean?

Basic idea

The term *one-body dissipation* does not mean that local equilibrium is instantaneously reached. It means that dissipation is generated by the action of the collective motion on the one-body phase-space distribution.

Collective motion

The time-dependent mean field acts as a moving container:

- the nuclear surface changes with time,
- single-particle motion is distorted,
- the intrinsic distribution is driven away from local equilibrium.

Loss of information

The distortion of the microscopic distribution can be partly randomized by:

- two-body collisions,
- stochastic parts of the one-body potential,
- chaotic single-particle motion in a moving nuclear cavity.

The macroscopic result is friction acting on the collective coordinates.

Knudsen-gas picture of nucleons

Long mean free path

At low and moderate excitation energies, Pauli blocking strongly suppresses two-body nucleon–nucleon collisions. Therefore, nucleons have a long mean free path and move almost freely inside the nuclear shape.

Nucleons as a Knudsen gas

The nucleus behaves like a finite Fermi gas in a moving container:

- particles move in the self-consistent mean field,
- the surface plays the role of a confining wall,
- collective motion changes the boundary conditions.

Why this matters

When the wall moves, the particle distribution near the surface is distorted. The mismatch between the wall velocity and the local drift velocity of the gas produces energy dissipation.

This provides the physical basis of the wall formula for nuclear friction.

Wall dissipation

Physical mechanism

Wall dissipation occurs when particles approaching the nuclear surface do not have the same normal velocity as the moving wall. After reflection, their velocity distribution is distorted relative to the bulk Fermi gas.

Rate of dissipated energy

For a moving surface element, the energy-loss rate is proportional to the square of the mismatch between the wall velocity and the local drift velocity:

$$\dot{Q}^{\mathrm{wall}} \propto \int_{\mathrm{surface}} df \left[\mathbf{n} \cdot (\mathbf{w} - \mathbf{v}_d)\right]^2 .$$

Meaning

- $\mathbf{w}$: velocity of the moving surface,
- $\mathbf{v}_d$: drift velocity of the intrinsic gas,
- $\mathbf{n}$: normal vector to the surface.

The more strongly the surface motion distorts the local Fermi sphere, the larger the friction.

In the Langevin equation this mechanism enters through the friction tensor $\gamma_{ij}^{\mathrm{wall}}$.

Wall friction tensor in collective coordinates

Friction force

If the dissipated energy is quadratic in collective velocities, the friction force can be written as

$$F_i = -\sum_j R_{ij}\dot{q}_j,$$

where R_{ij} is the friction tensor.

Wall contribution

For a shape described by collective coordinates q_i, the wall mechanism leads to a tensor of the form

$$R_{ij}^{\mathrm{wall}} \sim \rho_F \bar{v} \int_{\mathrm{surface}} df \, \frac{\partial R}{\partial q_i} \frac{\partial R}{\partial q_j},$$

or, in axial coordinates, to the familiar wall-friction expression used in Langevin calculations.

Important point

The tensor couples different collective modes. Therefore, dissipation is not only a scalar damping strength: it depends on the shape and on the direction of motion in deformation space.

Window friction near scission

Additional dissipation mechanism

When the system develops two nascent fragments connected by a neck, particles can pass through the window between them. This gives rise to the *window friction* mechanism.

Wall friction

- interaction with a moving outer surface,
- dominant for compact mononuclear shapes,
- related to distortion of the Fermi distribution near the wall.

Window friction

- exchange of particles through the neck,
- tends to equilibrate momentum distributions of nascent fragments,
- becomes important when a pronounced neck is formed.

In low-energy fission the relative velocity of the nascent fragments is small, so the window contribution may be less dominant than in heavy-ion collisions.

Dissipation, entropy, and model reduction

Why entropy depends on the model

The entropy attributed to the intrinsic system depends on which collective coordinates are treated explicitly. A more detailed collective model leaves less energy hidden in the intrinsic subsystem and can therefore produce less entropy.

Coarse-grained picture

A reduced model with only a few collective variables treats many degrees of freedom as intrinsic. This increases apparent irreversibility and friction.

Microscopic picture

A richer model resolves more collective modes explicitly. Some apparent dissipation may then be reinterpreted as motion in additional coordinates.

This is directly relevant to the too-narrow mass distributions obtained in restricted 3D fission dynamics.

Connection to the present Langevin calculations

Role in the model

The one-body dissipation picture motivates the friction tensor used in the Langevin equation:

$$\dot{p}_i = -\frac{\partial V}{\partial q_i} - \sum_{jk} \gamma_{ij}(\mathbf{q}, T)[m^{-1}(\mathbf{q})]_{jk} p_k + \sum_j g_{ij}(\mathbf{q})\Gamma_j(t) + \dots$$

Friction

$$\gamma_{ij}(\mathbf{q}, T)$$

controls how fast collective kinetic energy is converted into intrinsic excitation.

Fluctuations

The same coupling produces random forces through

$$\sum_k g_{ik} g_{jk} = \gamma_{ij} T^*.$$

Therefore, stronger dissipation also changes the diffusive exploration of the PES.

The competition between deterministic PES descent, friction, and fluctuations determines whether trajectories remain in asymmetric valleys or reach the symmetric valley.