Hirschegg 2012

Facets of Strong-Interaction Physics

15-21 January 2012, Hirschegg, Austria

Brownian shape motion: Fission fragment mass distributions

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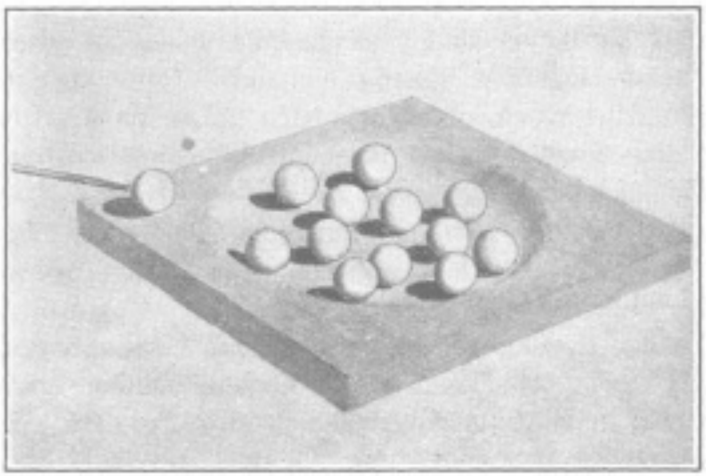
Basic concepts in fission

Nature 137 (1936) 351 quoting Niels Bohr:
``.. the energy of the incident neutron will be rapidly divided among all the nuclear particles ..''



Niels Bohr, Nature 143 (1939) 330:
``.. any nuclear reaction initiated by collisions or radiation involves as an intermediate stage the formation of a compound nucleus in which the excitation energy is distributed among the various degrees of freedom in a way resembling thermal agitation ..''

N. Bohr & J.A. Wheeler, Phys Rev 56 (1939) 426:

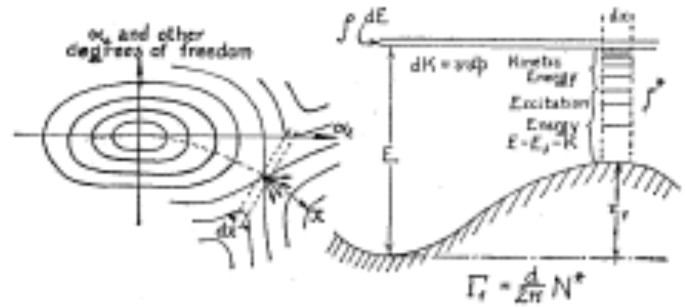


FIG. 3. The potential energy associated with any arbitrary deformation of the nuclear form may be plotted as a function of the parameters which specify the deformation, thus giving a contour surface which is represented schematically in the left-hand portion of the figure. The pass or saddle point corresponds to the critical deformation of unstable equilibrium. To the extent to which we may use classical terms, the course of the fission process may be symbolized by a ball lying in the hollow at the origin of coordinates (spherical form) which receives an impulse (neutron capture) which sets it to executing a complicated Lissajous figure of oscillation about equilibrium. If its energy is sufficient, it will in the course of time happen to move in the proper direction to pass over the saddle point (after which fission will occur), unless it loses its energy (radiation or neutron re-emission). At the right is a cross section taken through the fission barrier, illustrating the calculation in the text of the probability per unit time of fission occurring.

Standard framework for fission dynamics

Define a suitable parametrized family of nuclear shapes: $\boldsymbol{\chi} = \{\chi_i\}$

1) Calculate the potential energy of deformation: $U(\boldsymbol{\chi}) = U(\{\chi_i\})$

2) Calculate the inertial mass tensor: $K(\boldsymbol{\chi},\dot{\boldsymbol{\chi}}) = \frac{1}{2}\dot{\boldsymbol{\chi}} \cdot \boldsymbol{M}(\boldsymbol{\chi}) \cdot \dot{\boldsymbol{\chi}} = \frac{1}{2}\sum_{ij} \dot{\chi}_i M_{ij}(\boldsymbol{\chi})\dot{\chi}_j$

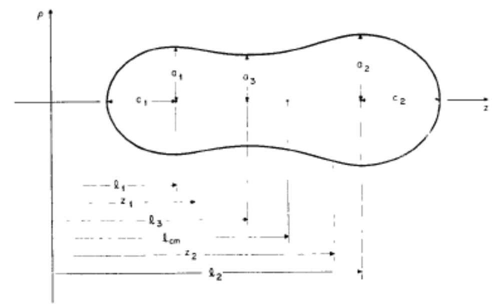
3) Calculate the friction tensor: $\mathcal{F}(\boldsymbol{\chi},\dot{\boldsymbol{\chi}}) = \frac{1}{2}\dot{\boldsymbol{\chi}} \cdot \boldsymbol{\gamma}(\boldsymbol{\chi}) \cdot \dot{\boldsymbol{\chi}} = \frac{1}{2}\sum_{ij} \dot{\chi}_i \gamma_{ij}(\boldsymbol{\chi})\dot{\chi}_j$

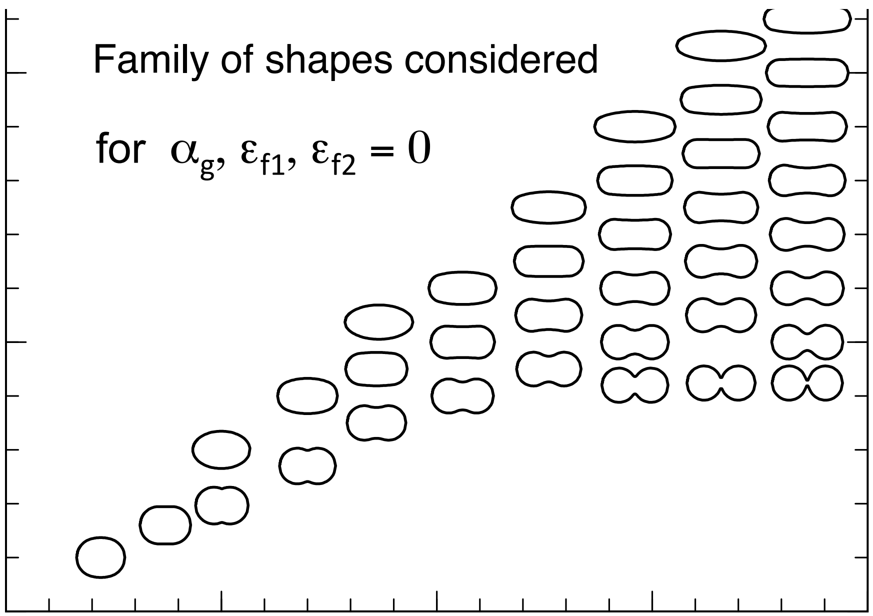
Solve the equations of motion: $\frac{d}{dt}\left(\frac{\partial \mathcal{L}}{\partial \dot{\chi}_i}\right) = \frac{\partial \mathcal{L}}{\partial \chi_i} - \frac{\partial \mathcal{F}}{\partial \dot{\chi}_i}$

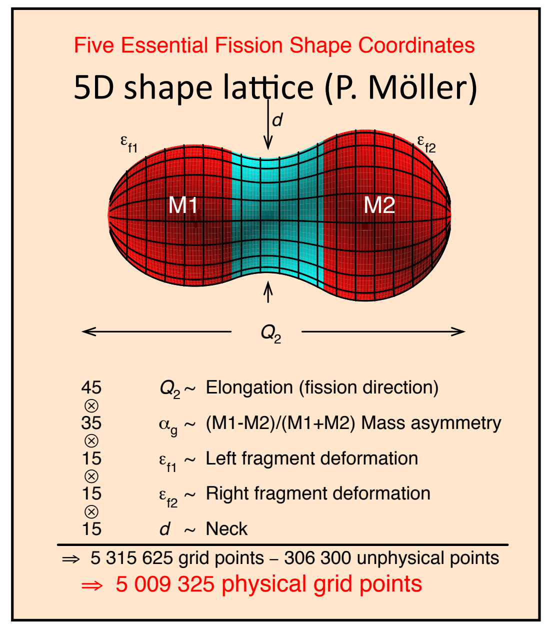
Add stochastic forces (dissipation => fluctuation): Γ_i

Nuclear shapes relevant for fission

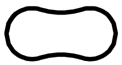
5D shape family:
3 quadratic surfaces of revolution
[J.R. Nix, NPA130 (1969) 241]







Nuclear potential energy of deformation

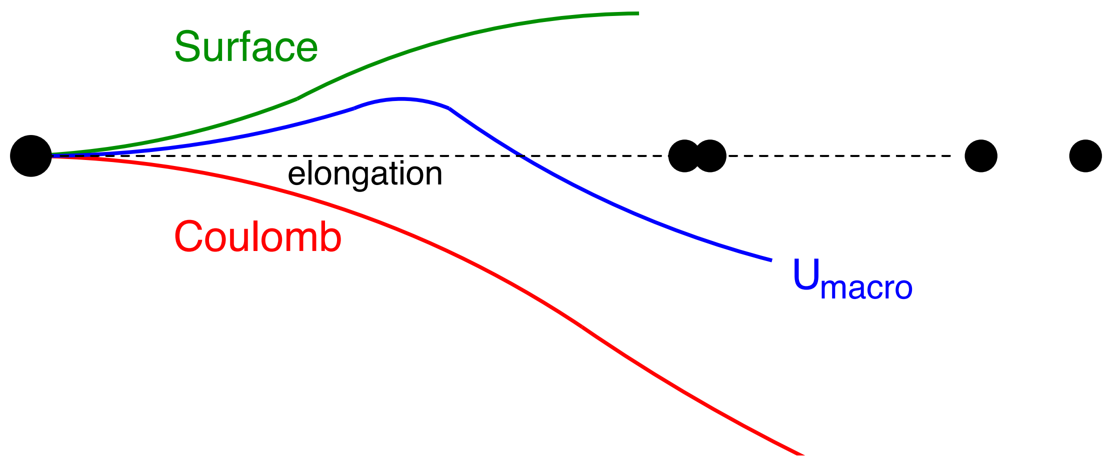


Macroscopic-microscopic method:

$$U_{total}(\text{shape}) = U_{macro}(\text{shape}) + U_{micro}(\text{shape})$$

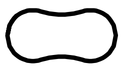
finite-range liquid drop

Strutinski procedure



$$U_{\text{macro}}(\text{shape}) = E_{\text{surf}}(\text{shape}) + E_{\text{Coul}}(\text{shape}) + \ldots$$

Nuclear potential energy of deformation

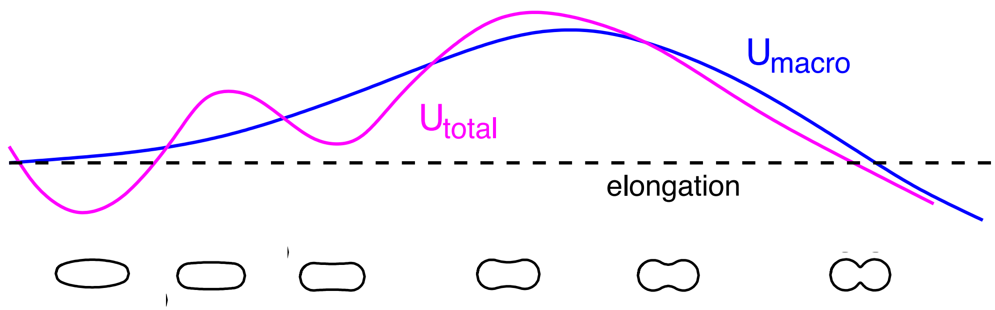


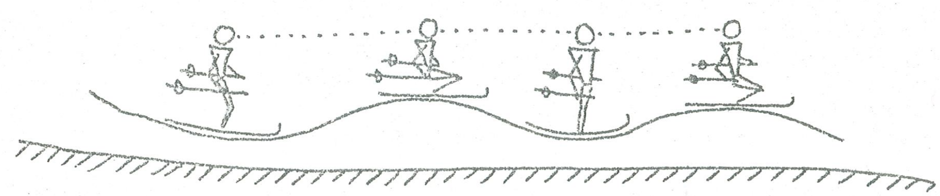
Macroscopic-microscopic method:

$$U_{total}(\text{shape}) = U_{macro}(\text{shape}) + U_{micro}(\text{shape})$$

finite-range liquid drop

Strutinski procedure

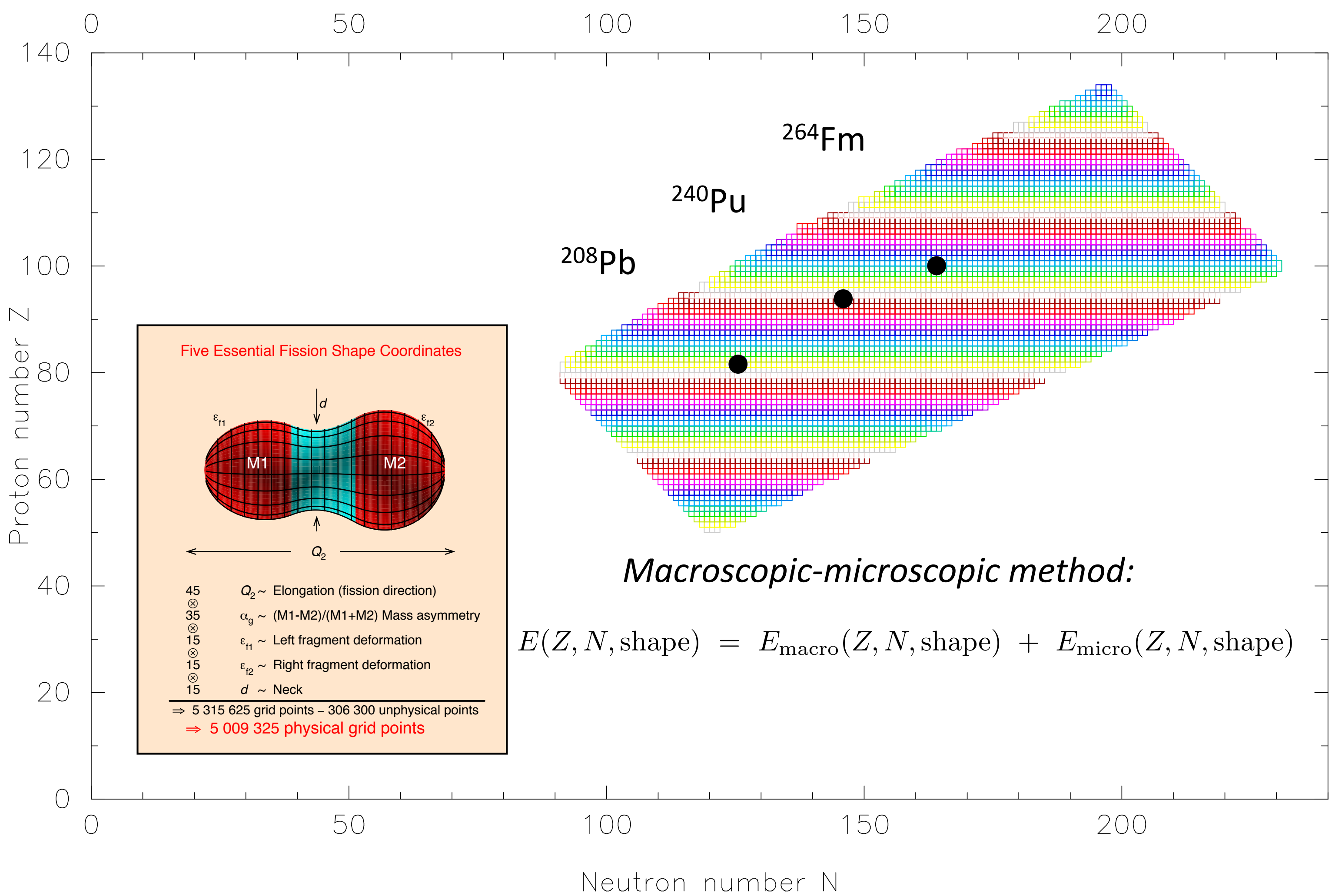




From summary of 2nd Hirschegg Winter Workshop by John Negele

5D deformation-energy surfaces for 5254 nuclei

P. Möller *et al*, Phys Rev C79, 064304 (2009)



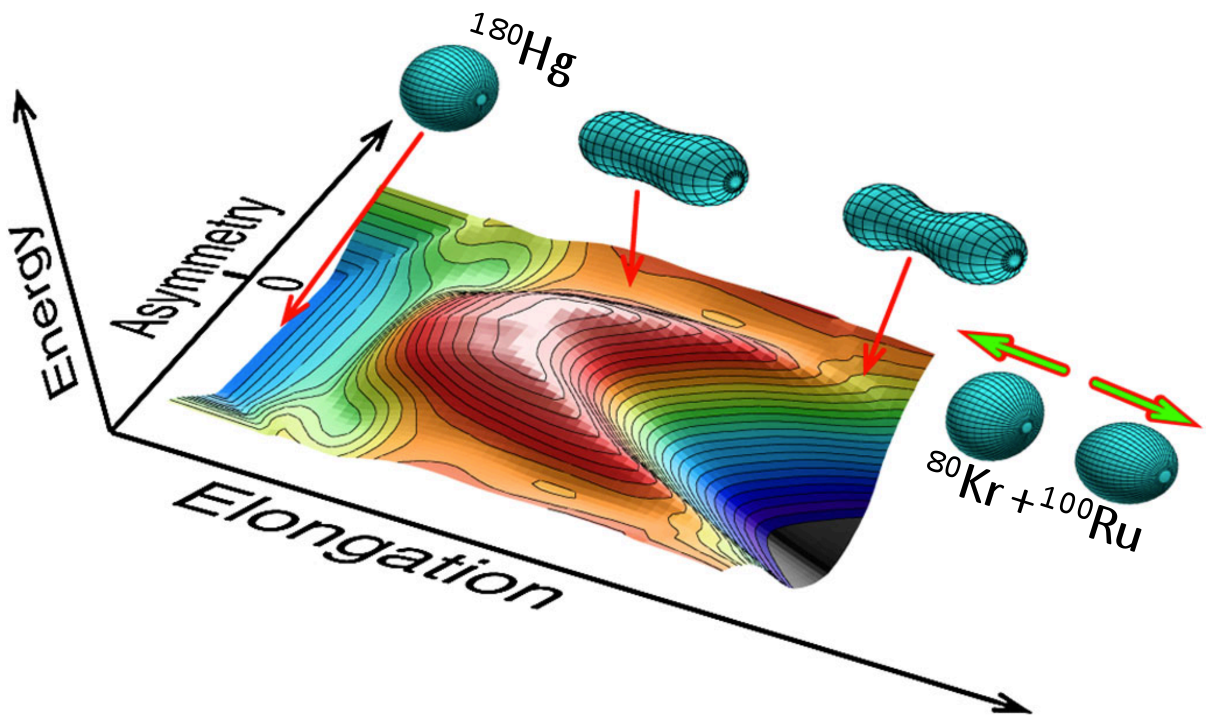
Macroscopic-microscopic method:

$$E(Z,N,\mathrm{shape}) = E_{\mathrm{macro}}(Z,N,\mathrm{shape}) + E_{\mathrm{micro}}(Z,N,\mathrm{shape})$$

Potential-energy surface for ^{236}U

(calculated by P. Möller 1970)

Example: Fission of ^{180}Hg



Adapted from plot made by T. Ichikawa for

A. Andreyev et al, Phys Rev Lett 105 (2010) 252502:
New type of asymmetric fission in proton-rich nuclei

Strongly damped nuclear shape dynamics: Brownian motion

Strong dissipation => creeping evolution => mass unimportant

Strongly damped EoM:

$$\boldsymbol{F}^{\rm pot} + \boldsymbol{F}^{\rm fric} + \boldsymbol{F}^{\rm ran} \doteq \mathbf{0}$$

Smoluchowski Equation

$$\left\{ \begin{array}{l} \boldsymbol{F}^{\rm pot} = -\partial U/\partial \boldsymbol{\chi} \\ \boldsymbol{F}^{\rm fric} = -\partial \mathcal{F}/\partial \dot{\boldsymbol{\chi}} = -\boldsymbol{\gamma}\cdot\dot{\boldsymbol{\chi}} \\ \langle \boldsymbol{F}^{\rm ran}(t)\rangle = \mathbf{0} \\ \langle F_i^{\rm ran}(t) F_j^{\rm ran}(t')\rangle \;=\; 2T\gamma_{ij}\delta(t-t') \end{array} \right.$$

Brownian motion

Solution:

$$\dot{\boldsymbol{\chi}} = \boldsymbol{\mu}\cdot(\boldsymbol{F}^{\rm pot} + \boldsymbol{F}^{\rm ran})$$

Mobility tensor: $\boldsymbol{\mu} \;\equiv\; \boldsymbol{\gamma}^{-1}$

=> Average shape evolution: $\dot{\bar{\chi}}_i \;\doteq\; \sum_j \mu_{ij} F_j^{\rm pot}$ $\qquad \mu_{ij} \;=\; \sum_n \tilde{\chi}_i^{(n)} \tilde{\chi}_j^{(n)}$

Direct numerical simulation: $\delta\chi_i \;=\; \sum_n \tilde{\chi}_i^{(n)} \left[\Delta t\, \tilde{\boldsymbol{\chi}}^{(n)}\cdot \boldsymbol{F}^{\rm pot} + \sqrt{2T\Delta t}\,\xi_n\right]$

➔ *Isotropic mobility => simple random walk on the lattice => Metropolis*

Random walk on the 5D potential-energy landscape

Metropolis method:

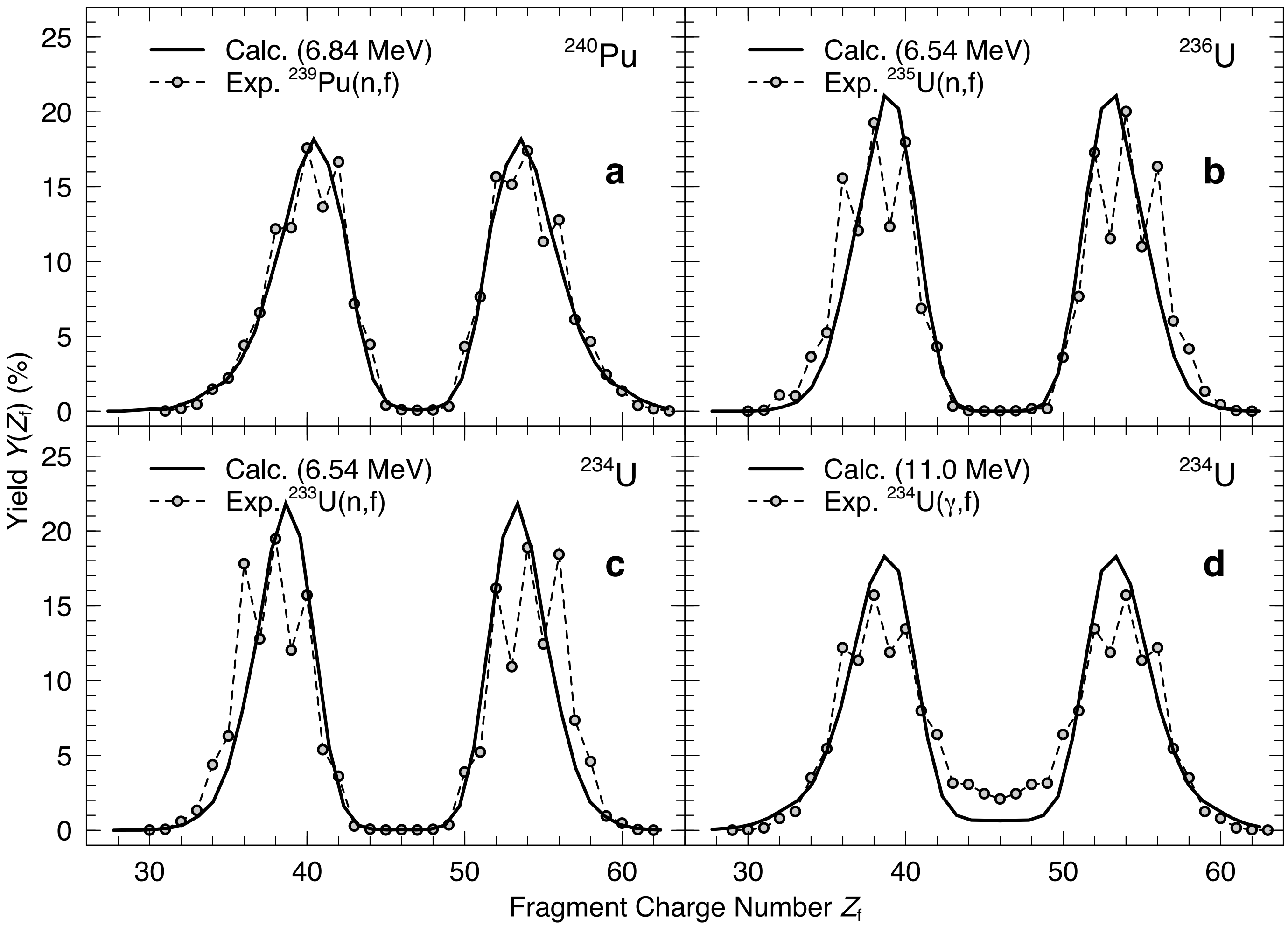
(to step or not to step?)

$$\Delta U = U' - U: \begin{cases} \Delta U < 0: & P(step) = 1 \\ \Delta U > 0: & P(step) = \exp(-\Delta U/T) \end{cases}$$


Random walk in the Hirschegg landscape
X marks
the target

$P(A_f)$ from $^{240}Pu^*$ and $^{236,234}U^*$

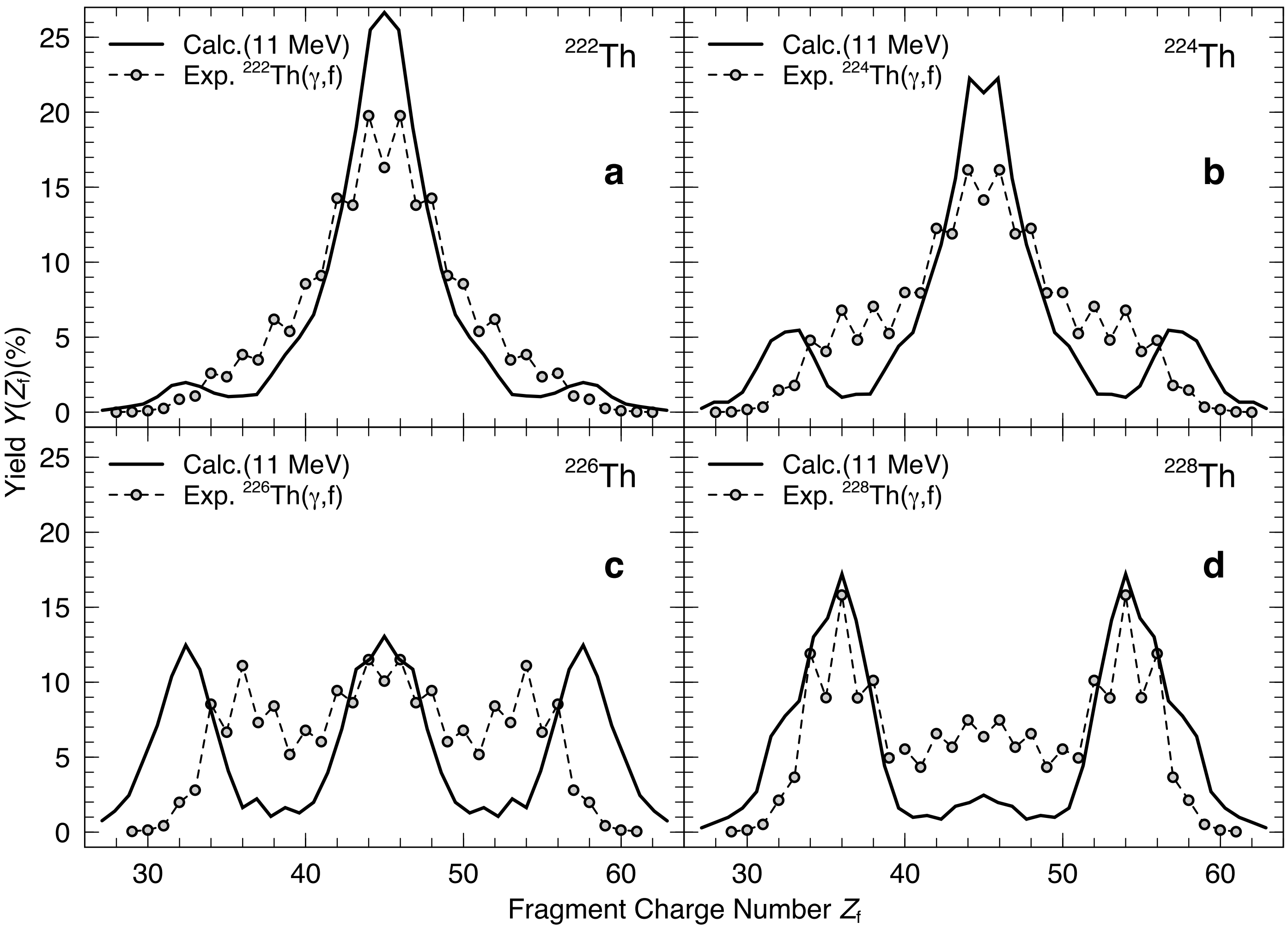
5D Metropolis walks



J. Randrup & P. Möller, PRL 106 (2011) 132503

$P(A_f)$ for $^{222,224,226,228}Th(\gamma,f)$

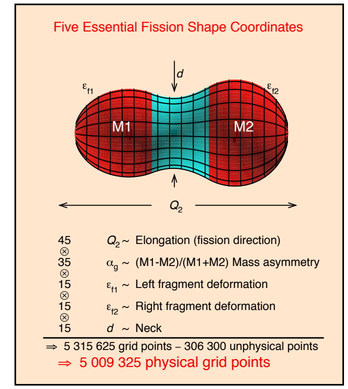
5D Metropolis walks



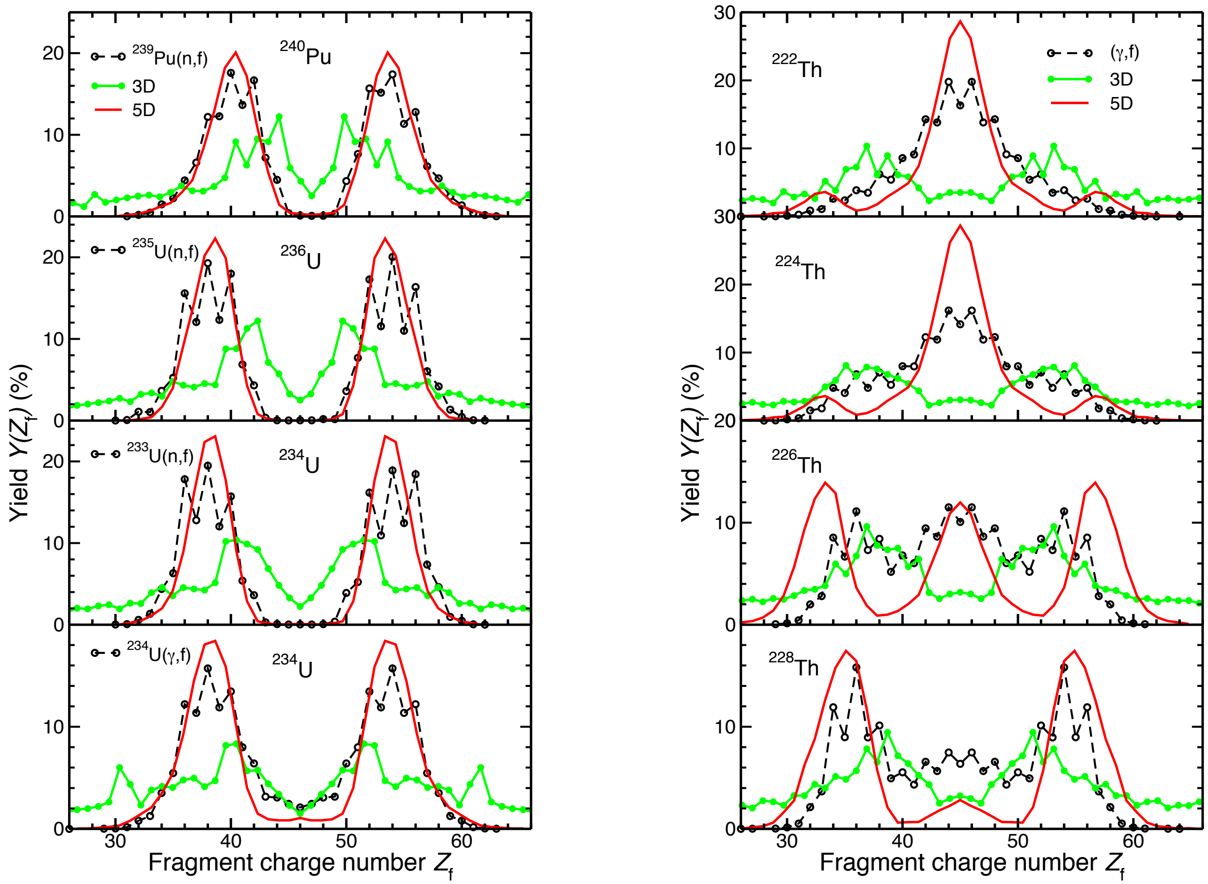
J. Randrup & P. Möller, PRL 106 (2011) 132503

JR, P. Möller, A.J. Sierk,
PRC 84 (2011) 034613

Restricted shape family?



5D -> 3D: $V(i,j,m) = \min_{kl}[V(i,j,k,l,m)]$



=> Must use sufficiently flexible shapes!

Brownian nuclear shape motion

Smoluchowski Equation)*

$$\dot{\boldsymbol{\chi}} = \boldsymbol{\mu} \cdot (\boldsymbol{F}^{\text{pot}} + \boldsymbol{F}^{\text{ran}})$$

$$\begin{cases} \boldsymbol{F}^{\text{pot}} = -\partial U / \partial \boldsymbol{\chi} \\ \boldsymbol{F}^{\text{fric}} = -\partial \mathcal{F} / \partial \dot{\boldsymbol{\chi}} = -\boldsymbol{\gamma} \cdot \dot{\boldsymbol{\chi}} \\ \langle \boldsymbol{F}^{\text{ran}}(t) \rangle = \mathbf{0} \\ \langle F_i^{\text{ran}}(t) F_j^{\text{ran}}(t') \rangle = 2T \gamma_{ij} \delta(t - t') \end{cases}$$

Mobility tensor: $\boldsymbol{\mu} \equiv \boldsymbol{\gamma}^{-1}$

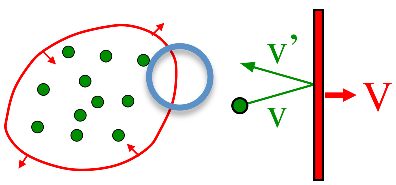
$$\mu_{ij} = \sum_n \tilde{\chi}_i^{(n)} \tilde{\chi}_j^{(n)}$$

*) Solve EoM by direct numerical simulation:

$$\delta \chi_i = \sum_n \tilde{\chi}_i^{(n)} \left[\Delta t \, \tilde{\boldsymbol{\chi}}^{(n)} \cdot \boldsymbol{F}^{\text{pot}} + \sqrt{2T \Delta t} \, \xi_n \right]$$

Nuclear one-body dissipation

.. in the mononucleus:



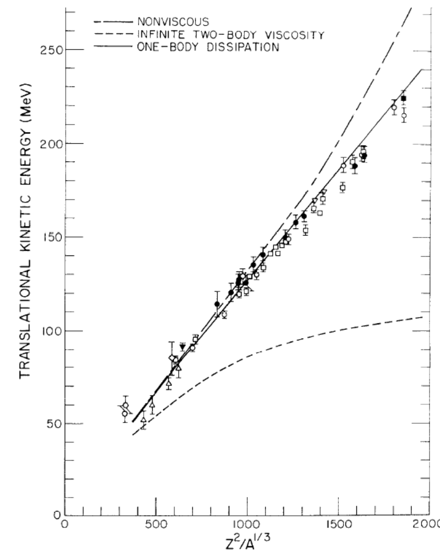
v'=2V−v

Ann Phys **113** (1978) 330

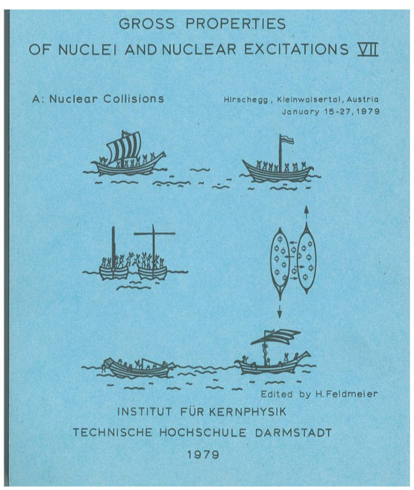
Wall dissipation fromula:

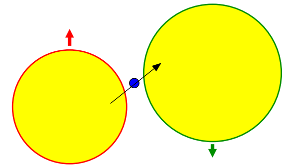
$$\dot{Q} \;=\; m\rho_0\bar{v}\oint d^2\sigma\,\dot{n}^2$$

.. is strong (and ~constant)



.. in the dinucleus:



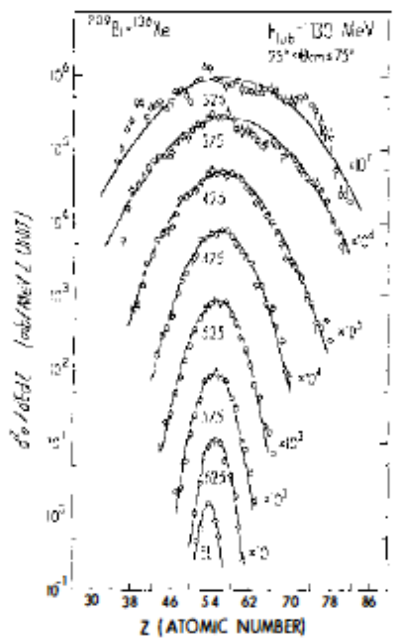


$$Q \;\sim\; V_{AB} v_F \mathcal{N}$$

$Q = -\Delta E_{\rm rel}$ Dissipated energy

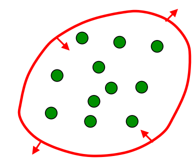
$\mathcal{N} = \sigma_A^2$ Nucleons exchanged

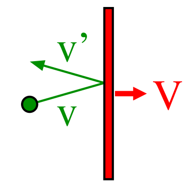
Nucl Phys **A307** (1978) 319; **A327** (1979) 490



Ann Rev Nucl Sci 27, 465 (1977)

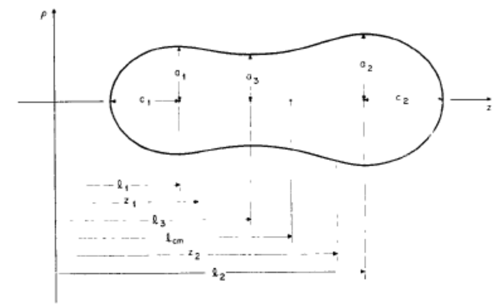
Structure of the mobility tensor?





Dissipation rate:
1b wall formula

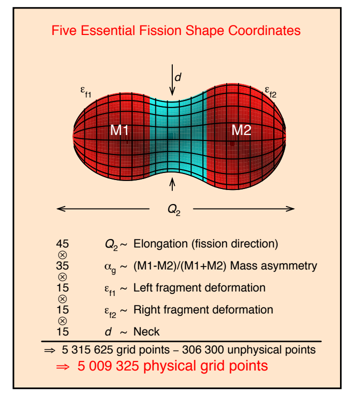
$$\dot{Q} = m\rho_0\bar{v} \oint d^2\sigma\, \dot{n}^2$$



$$\dot{Q} = \sum_{ij} \dot{\chi}_i\, \gamma_{ij}(\boldsymbol{\chi})\, \dot{\chi}_i = \sum_{\mu\nu} \dot{q}_\mu\, \mathrm{g}_{\mu\nu}(\boldsymbol{q})\, \dot{q}_\nu$$

Friction tensor in the Nix variables:

$$\mathrm{g}_{\mu\nu} = \tfrac{\pi}{2} m\rho_0\bar{v} \int \frac{\partial\rho^2(z)}{\partial q_\mu} \frac{\partial\rho^2(z)}{\partial q_\nu} \left[\rho^2(z) + \tfrac{1}{4}\left(\frac{\partial\rho^2}{\partial z}\right)^2\right]^{-\frac{1}{2}} dz$$



Friction tensor γ in the lattice variables:

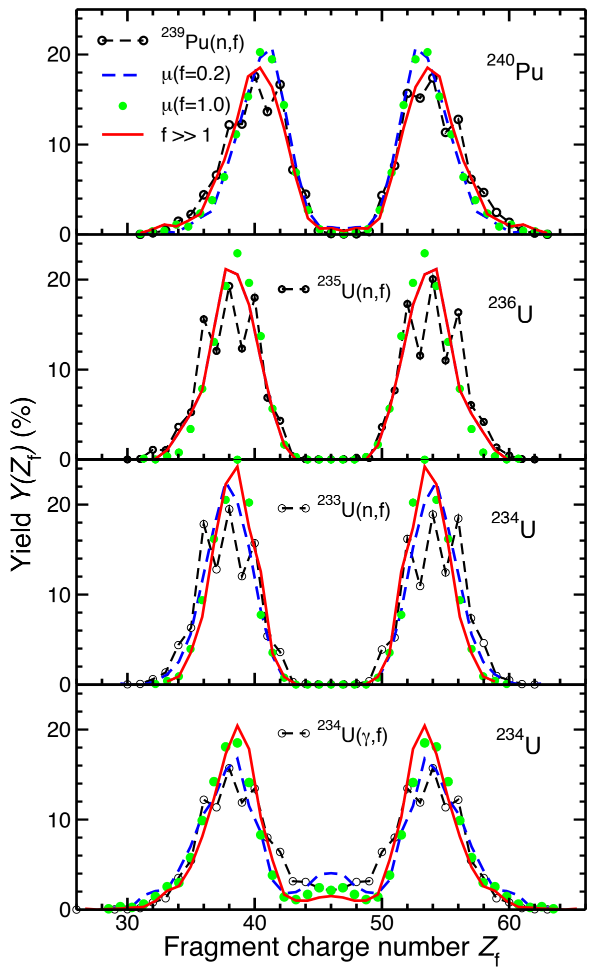
$$\gamma_{ij}(\boldsymbol{\chi}) = \sum_{\mu\nu} \frac{\partial q_\mu}{\partial \chi_i}\, \mathrm{g}_{\mu\nu}(\boldsymbol{q})\, \frac{\partial q_\nu}{\partial \chi_j}$$

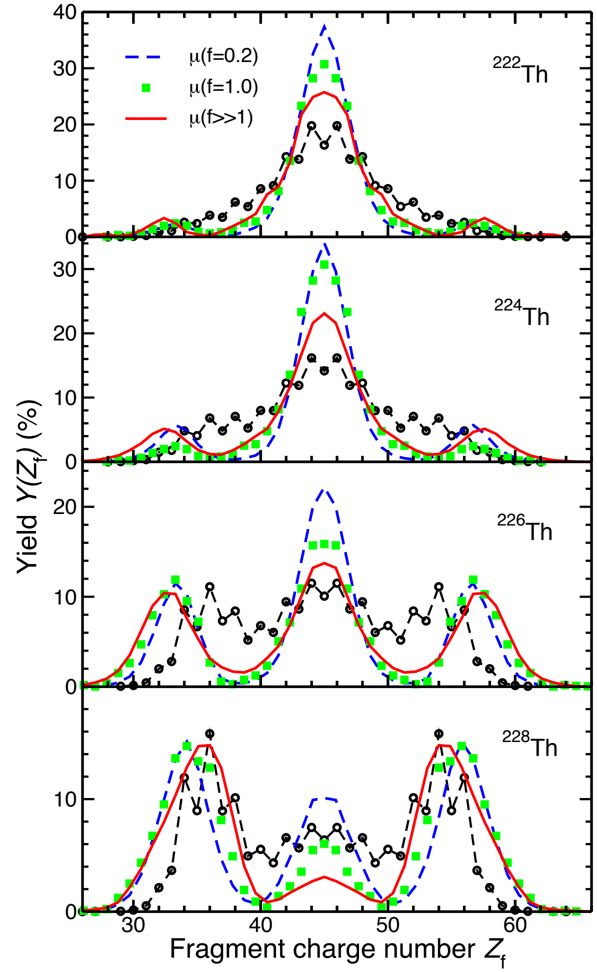
Isotropize γ at each lattice site:
$0 \leq f \leq \infty$

$$\tilde{\gamma}(f):\ \ \tilde{\gamma}_n(f) \equiv \frac{\gamma_n + f\overline{\gamma}}{1+f} \quad \text{where} \quad \overline{\gamma} \equiv \frac{1}{D}\sum_{n=1}^{D} \gamma_n$$

Dependence of $P(A_f)$ on the mobility tensor

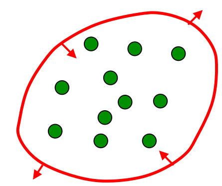
$$\tilde{\boldsymbol{\gamma}}(f):\ \ \tilde{\gamma}_n(f)\ \equiv\ \frac{\gamma_n + f\overline{\gamma}}{1+f} \quad \Rightarrow \quad \tilde{\boldsymbol{\mu}}(f)\ =\ \tilde{\boldsymbol{\gamma}}(f)^{-1} \qquad f = 0.2,\ 1.0,\ \infty$$





Main points:

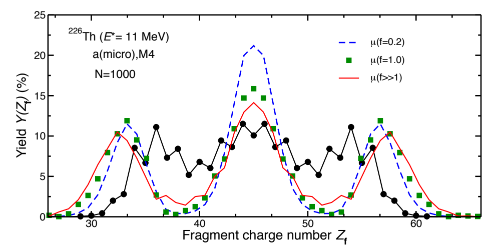
Shape motion is strongly damped => ignore inertial masses
=> Smoluchowski equation (Brownian motion)



$$\dot{\chi} = \boldsymbol{\mu} \cdot (\boldsymbol{F}^{\mathrm{pot}} + \boldsymbol{F}^{\mathrm{ran}})$$

$P(A_f)$ depends only weakly on the dissipation tensor
=> Metropolis walk is a reasonable starting point

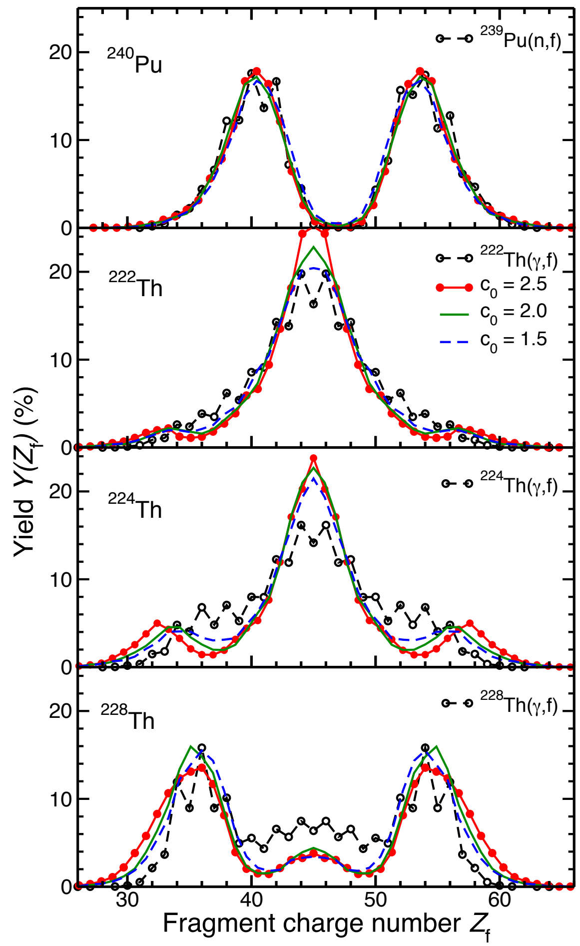
The dependence on the dissipation anisotropy provides an estimate of the uncertainty on the calculated $P(A_f)$



Metropolis walk:

The shape evolves until the neck has shrunk to a specified value c_0

Shape diffusion: *robust* wrt c_0

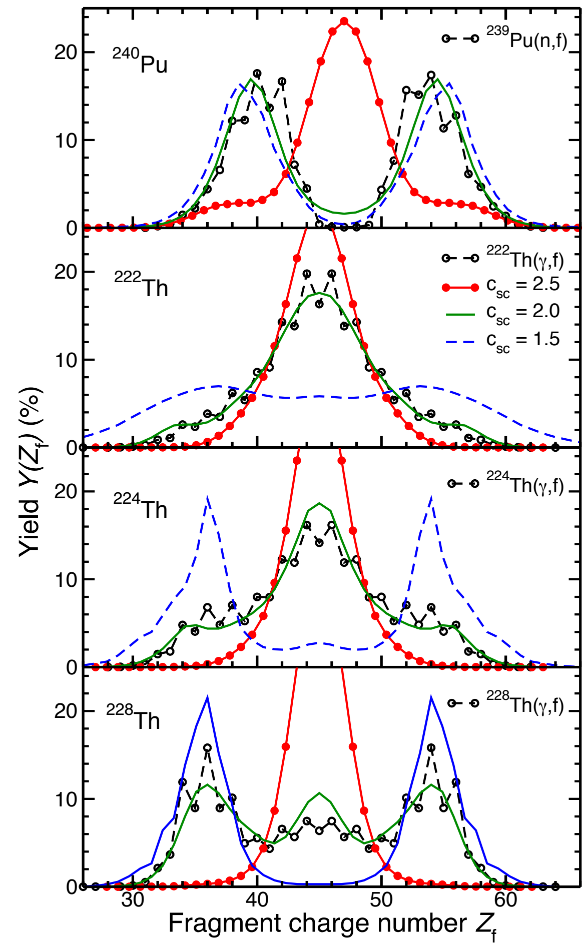


⇒ Shape dynamics on the pre-scission potential landscape is important!

Statistical scission:

*Each scission configuration is populated in proportion to its statistical weight**

Scission model: *sensitive* to c_{sc}



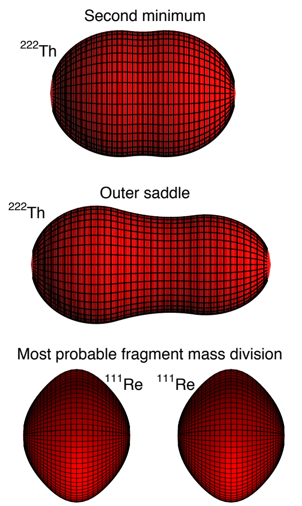
* Fong, Phys Rev 102 (1956) 434;
Wilkins et al, PRC 14 (1976) 1832

^{222}Th: Mass asymmetry is NOT determined at the saddle!

Q_2:

I=7

I=20

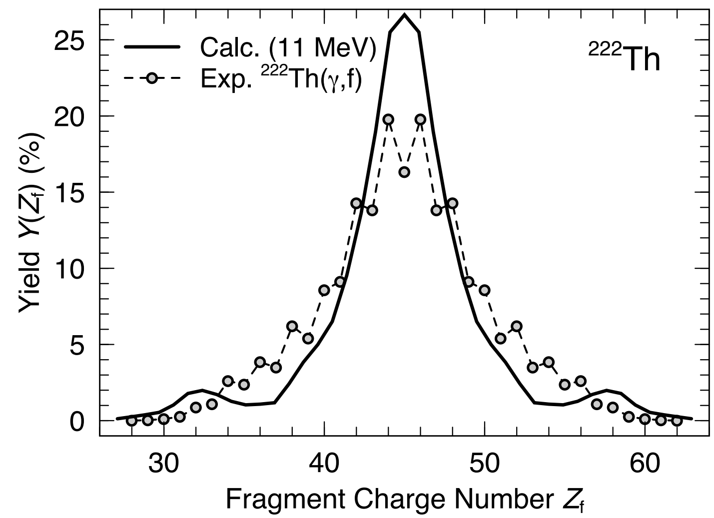


A_f:

M=0

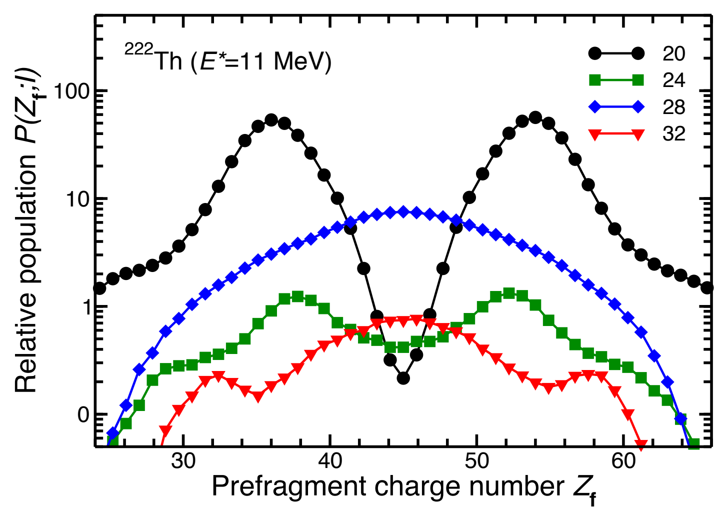
M=8

M=0



Distribution of mass asymmetries at a specified fixed elongation Q_2:

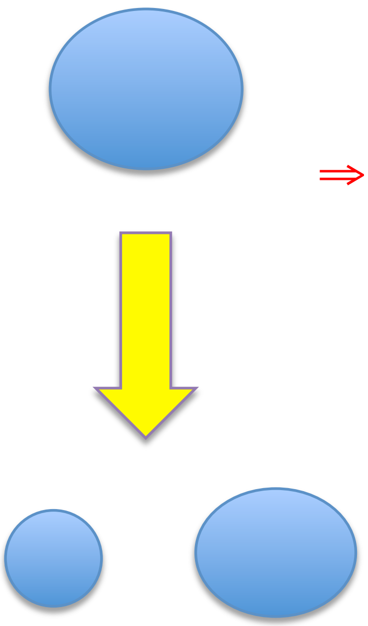
$$P(A_{\rm f};Q_2)\ \sim \prec \sum_n \delta(I_n - I)\,\delta(M_n - M) \succ$$



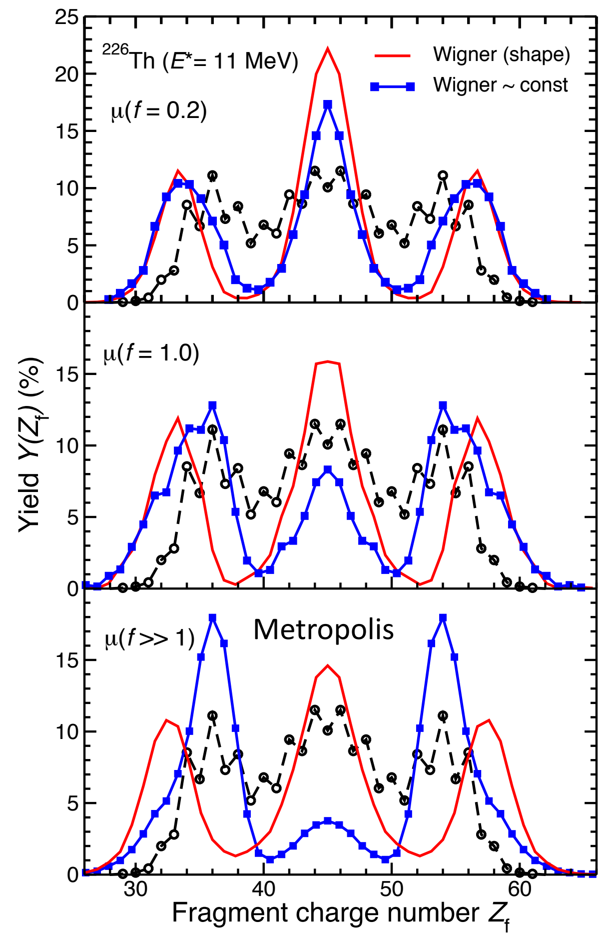
^{226}Th: Shape dependence of the Wigner term?

$$E(Z,N,\text{shape}) \; = \; E_{\text{macro}}(Z,N,\text{shape}) \; + \; E_{\text{micro}}(Z,N,\text{shape})$$

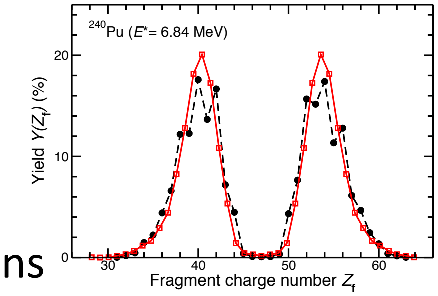
$$E_{\text{macro}}(Z,N,\text{shape}) \; = \; \cdots \; + \; W(\text{shape}) \, \frac{|N-Z|}{A}$$



$\Rightarrow$ *The shape dependence of the Wigner term influences $P(A_f)$!*



Summary and perspectives



Novel model for calculating fission fragment mass distributions

Augments the standard compound nucleus picture with explicit simulation of the equilibration *dynamics*

Conceptually very simple

Required:

- The deformation-energy landscape for a *sufficiently rich* family of fission shapes

  Very important

- The friction tensor for the shape motion

  Less crucial

Unprecedented *predictive power*

Useful tool

Preliminary application possible to >5,000 nuclei for which the 5D surfaces are already available

Light Hg isotopes; end of *r*-process?

Requires only relatively *modest* computing power

~500,000 CPU hours vs ~minutes on a mac

A number of model aspects need further study

Friction tensor, energy dependence, ..

Extensions anticipated

Spontaneous fission? fragment TKE? …