Fission **E**xperiment**S** and **T**heoretical **A**dvances

Santa Fe, New Mexico, 8-12 September 2014

Lectures on Fission Dynamics
within the Macroscopic-Microscopic Approach

Jørgen Randrup

LBNL, Berkeley, California

BERKELEY LAB
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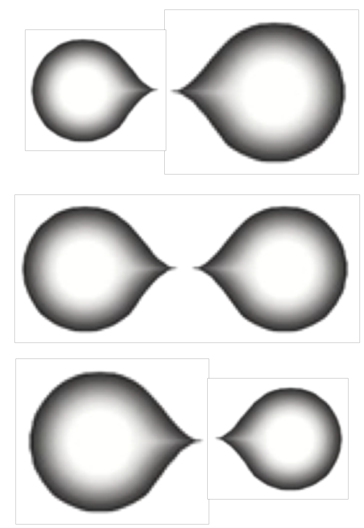

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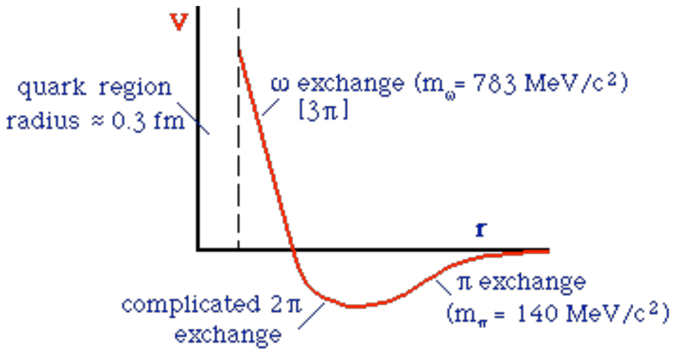
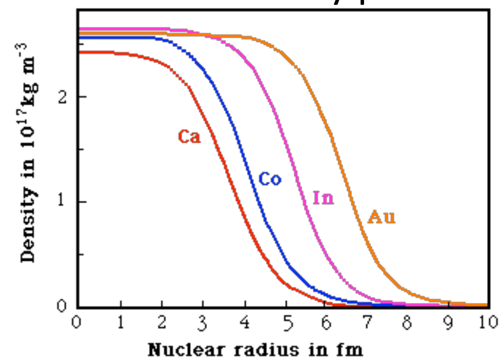
Basic features of nuclei: saturation

NN interaction

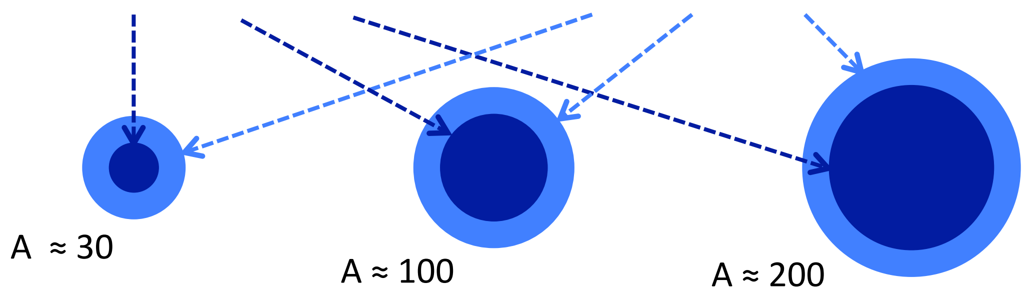


Nuclear density profiles



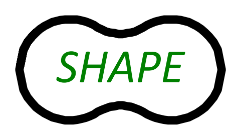
Same bulk density

Same surface profile



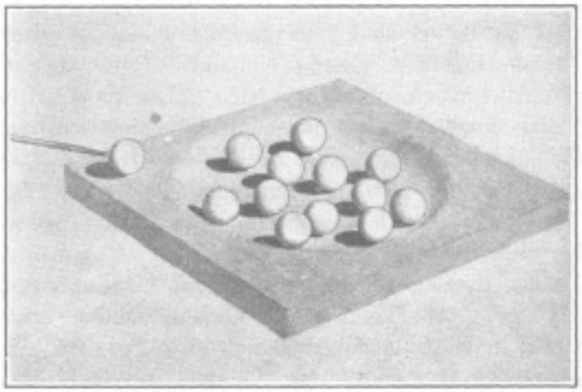
Nuclear matter *saturates*: $R \approx A^{1/3}$

Nuclei are *leptodermous*: $w << R$



Basic features of nuclei: memory loss

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

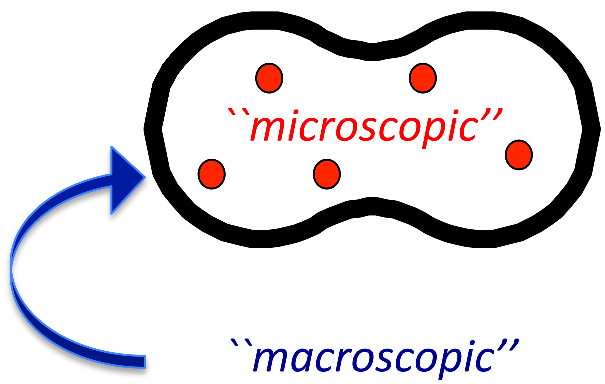


Niels Bohr, Nature 137 (1936) 344:
``.. neutron capture .. will result in .. the formation of a compound system of remarkable stability. The possible later breaking up of this system .. must in fact be considered as separate competing processes which have no immediate connexion with the first stage ..''

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 ..''

The internal relaxation is much faster than the evolution of the shape

$\tau_{\mathrm{micro}} \ll \tau_{\mathrm{macro}}$



-> *Evaporation*

-> *Fission*

Basic features of nuclear fission: shape dynamics

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

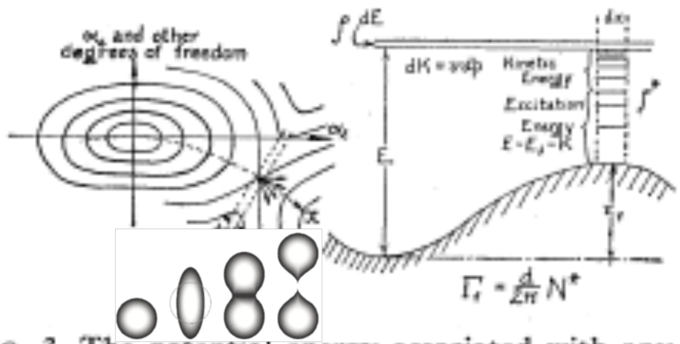


FIG. 3. The potential energy associated with any arbitrary deformation of the nuclear form may be plotted as a function of the parameters which specify the deformation, thus giving a contour surface which is represented schematically in the left-hand portion of the figure. The pass or saddle point corresponds 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.

Nuclear shape dynamics

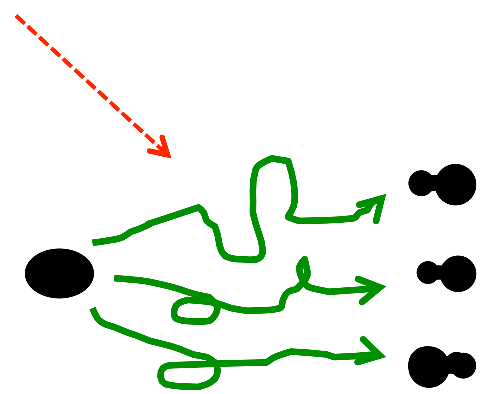
1) Parametrized family of nuclear shapes: $\boldsymbol{q} = \{q_i\}$  *N*

2) Potential energy of deformation: $U(\boldsymbol{q}) = U(q_1, q_2, \ldots)$ *1*

3) Inertial mass tensor: $\boldsymbol{M}(\boldsymbol{q}) = \{M_{ij}(\boldsymbol{q})\}$ *N x N*

4) Dissipation tensor: $\gamma(\boldsymbol{q}) = \{\gamma_{ij}(\boldsymbol{q})\}$ *N x N*

Langevin equation of motion: $d\boldsymbol{p}/dt = \boldsymbol{F}^{cons} + \boldsymbol{F}^{diss}$



Examples (incomplete list) [all macroscopic]:

Kramers, Physica 7 (1940) 284, …

Fröbrich & Gontchar, Phys Rep 292 (1998) 131

Chadhuri & Pal, Phys Rev C63 (2001) 064603

Karpov, Nadtouchy, Vanin, Adeev, Phys Rev C63 (2001) 054610

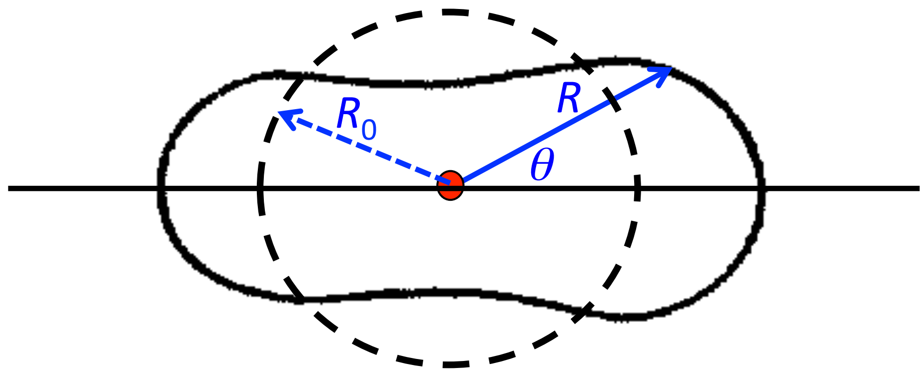
Nadtouchy, Adeev, Karpov, Phys Rev C65 (2002) 064615

Nadtouchy, Kelic, Schmidt, Phys Rev C75 (2007) 064614

Nuclear shape families

Axially symmetric nuclear shapes

Expansion of *R(θ)* on Legendre polynomials



$$R(\vartheta) \;=\; R_0 \left[1 + \sum_{n \geq 1} \alpha_n P_n(\vartheta) \right] / \lambda(\alpha_1, \alpha_2, \ldots)$$

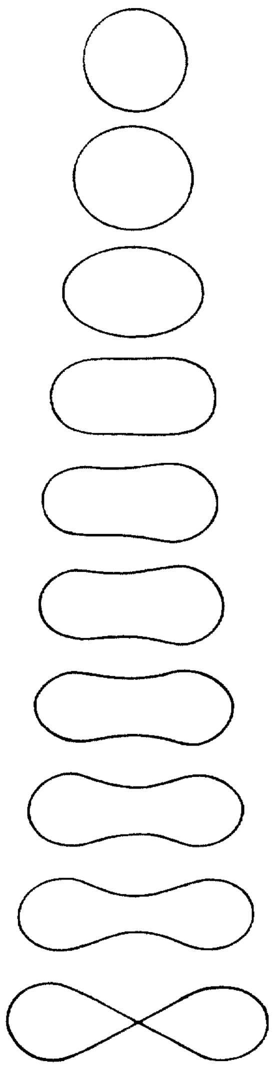
Very convenient for small deformations,
but unsuitable for large deformations!

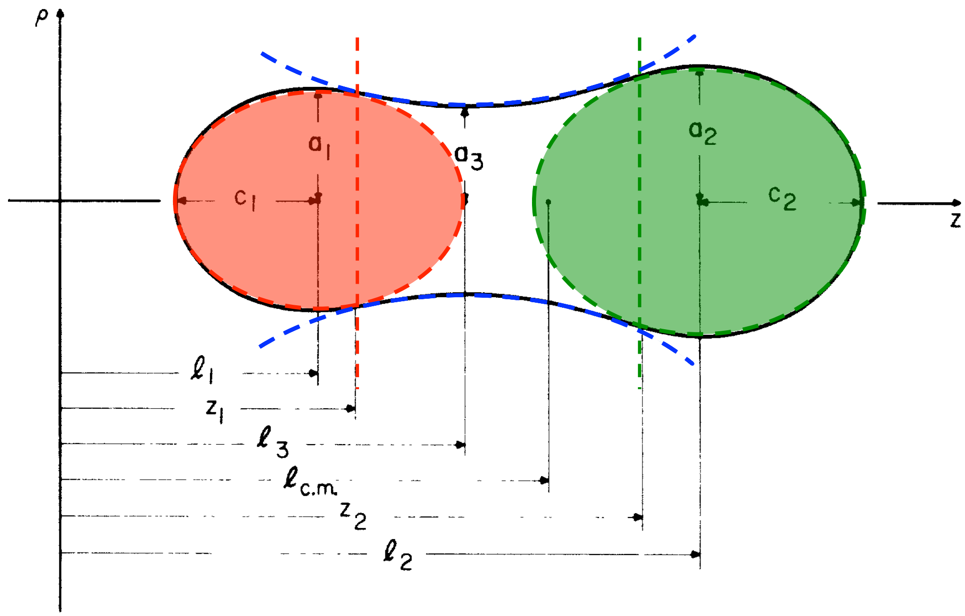
λ: Normalization constant
(to conserve the volume)

Nuclear shape families

Three quadratic surfaces [Nix 1968]

5 independent shape parameters





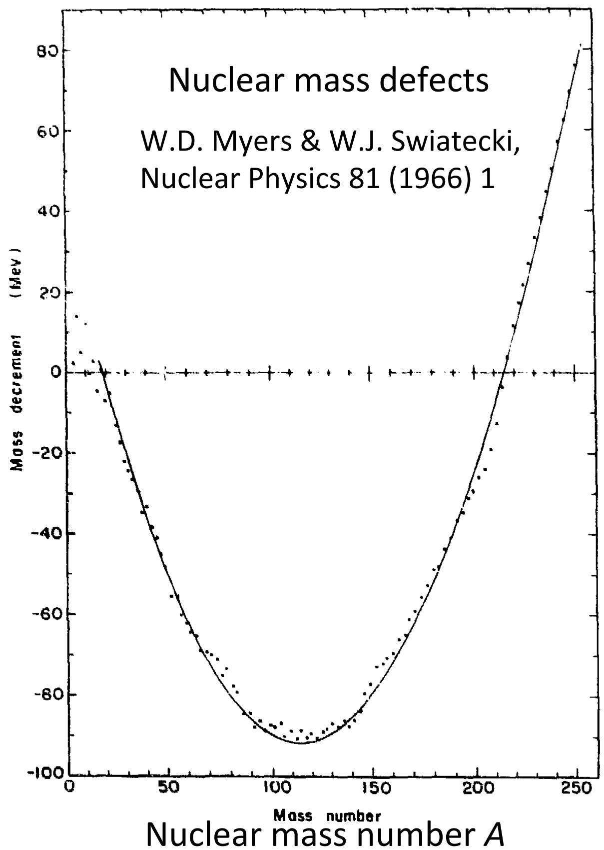
$z_0 < z < z_1$: $\rho(z)^2 = a_1^2 - (a_1^2/c_1^2)(z-l_1)^2$ spheroid

$z_1 < z < z_2$: $\rho(z)^2 = a_3^2 - (a_3^2/c_3^2)(z-l_3)^2$ spheroid/hyperboloid

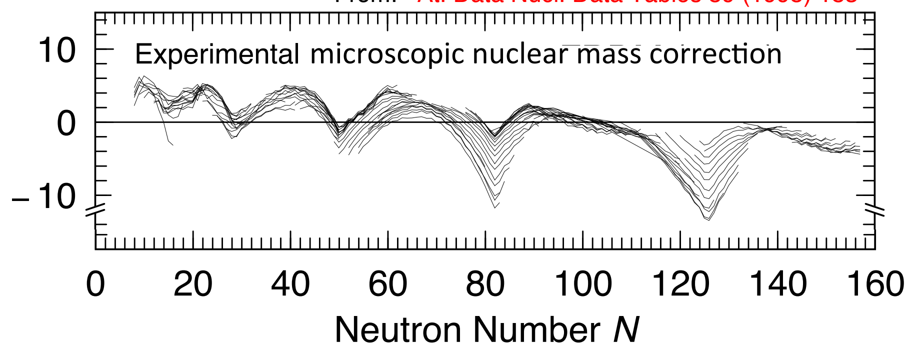
$z_2 < z < z_3$: $\rho(z)^2 = a_2^2 - (a_2^2/c_2^2)(z-l_2)^2$ spheroid

Nuclear potential energy: masses

The nuclear energy exhibits a smooth average plus
small deviations reflecting specific nuclear structure

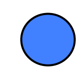


From: At. Data Nucl. Data Tables 59 (1995) 183

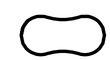


Liquid-drop mass formula [C.F. von Weizsäcker (1935)]:

$$M_{\text{macro}}(Z,A) \; = \; c_{\text{bulk}}A + c_{\text{surf}}A^{2/3} + c_{\text{coul}}Z^2/A^{1/3} + c_{\text{symm}}(N\text{-}Z)^2/A$$



Finite-range liquid-drop model (Nix, …)
and many others …



Nuclear potential energy: decomposition

The nuclear energy exhibits a smooth average plus small deviations reflecting specific nuclear structure

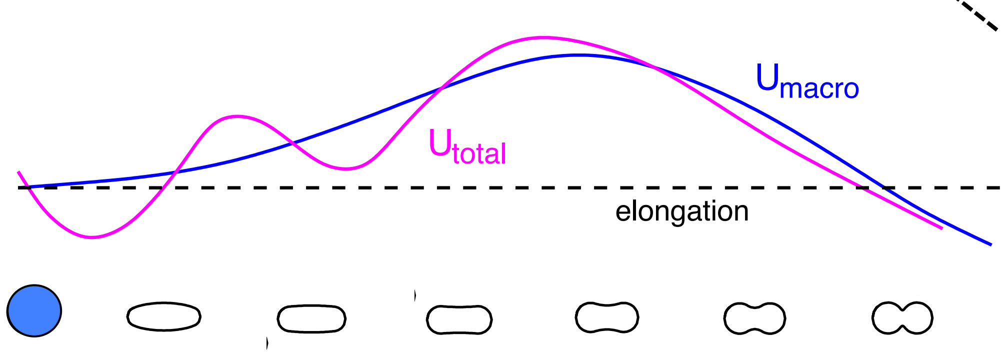
macroscopic: liquid drop | *microscopic:* shell+pairing

General: $U(Z,N,\ ) = E_{macro}(Z,N,\ ) + E_{s+p}(Z,N,\ )$

Swiatecki 1963
Strutinsky 1966

Masses: $M(Z,N,\ ) = M_{macro}(Z,N,\ ) + M_{micro}(Z,N,\ )$

mass relative to a macroscopic sphere



Nuclear potential energy: Macroscopic energy

Finite-Range Liquid-Drop Model

At. Data Nucl. Data Tables 59 (1995) 183

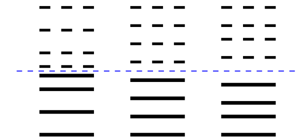
$E_{\rm macro}(Z,N,{\rm shape})\ =$

$M_{\rm H}Z+M_{\rm n}N$	mass excesses of Z hydrogen atoms and N neutrons
$-a_{\rm v}(1-\kappa_{\rm v}I^2)A$	volume energy
$+a_{\rm s}(1-\kappa_{\rm s}I^2)B_1({\rm shape})A^{2/3}$	surface energy
$+a_0A^0$	A^0 energy
$+c_1Z^2/A^{1/3}\,B_3({\rm shape})$	Coulomb energy
$-c_4Z^{4/3}/A^{1/3}$	Coulomb exchange correction
$+f(k_{\rm F}r_{\rm p})\,Z^2/A$	proton form–factor correction to Coulomb energy
$-c_{\rm a}(N-Z)$	charge–asymmetry energy
$+W\left(\lvert I\rvert+\begin{cases}1/A, & Z=N\ {\rm odd}\\ 0\,, & {\rm otherwise}\end{cases}\right)\times B_{\rm W}({\rm shape})$	Wigner energy
$+\begin{cases}\overline{\Delta}_{\rm p}+\overline{\Delta}_{\rm n}-\delta_{\rm np}, & Z\ {\rm and}\ N\ {\rm odd}\\ \overline{\Delta}_{\rm p}\,, & Z\ {\rm odd},\ N\ {\rm even}\\ \overline{\Delta}_{\rm n}\,, & Z\ {\rm even},\ N\ {\rm odd}\\ 0\,, & Z\ {\rm and}\ N\ {\rm even}\end{cases}$	average pairing energy
$-a_{\rm el}Z^{2.39}\,.$	energy of Z bound electrons

$$B_1({\rm shape}) = \frac{1}{8\pi^2R_0^2a^4}\int_V d^3\boldsymbol{r}\int_V d^3\boldsymbol{r}'\left(2-\frac{|\boldsymbol{r}-\boldsymbol{r}'|}{a}\right)\frac{{\rm e}^{-|\boldsymbol{r}-\boldsymbol{r}'|/a}}{|\boldsymbol{r}-\boldsymbol{r}'|/a} \qquad \approx 1 + (2/45)\,e^4$$

$$B_3({\rm shape}) = \frac{15}{32\pi^2R_0^5}\int_V d^3\boldsymbol{r}\int_V d^3\boldsymbol{r}'\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\left[1-\left(1+\tfrac{1}{2}\frac{|\boldsymbol{r}-\boldsymbol{r}'|}{a_{\rm den}}\right){\rm e}^{-|\boldsymbol{r}-\boldsymbol{r}'|/a_{\rm den}}\right] \qquad \approx 1 - (1/45)\,e^4$$

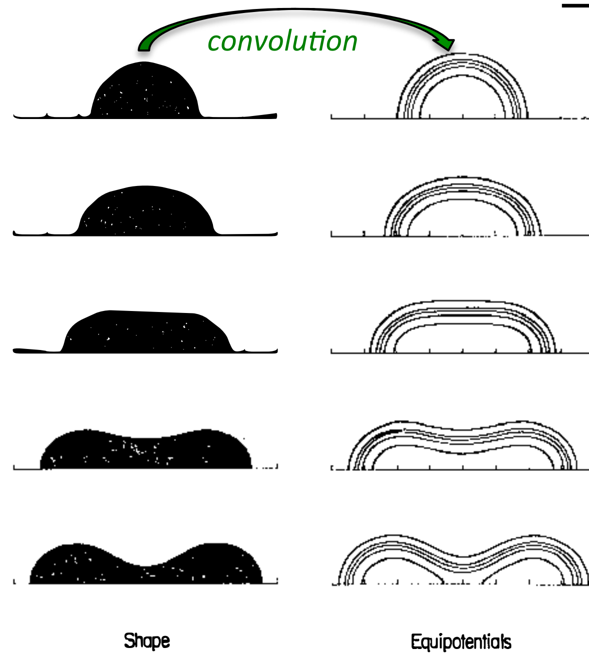
Nuclear potential energy: single-particle levels



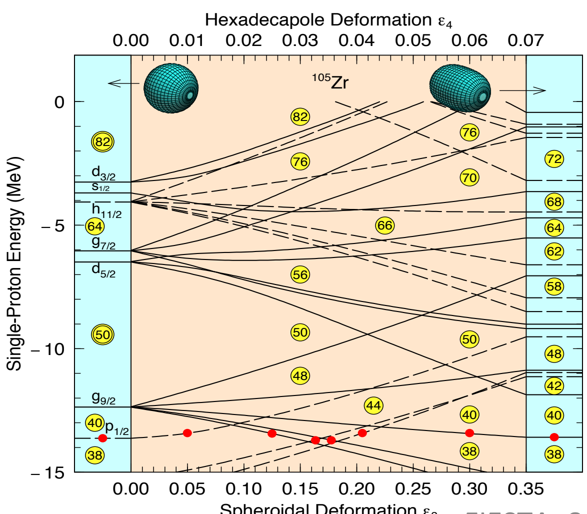
For a specified shape, generate the effective single-particle potentials for neutrons and protons by convolution

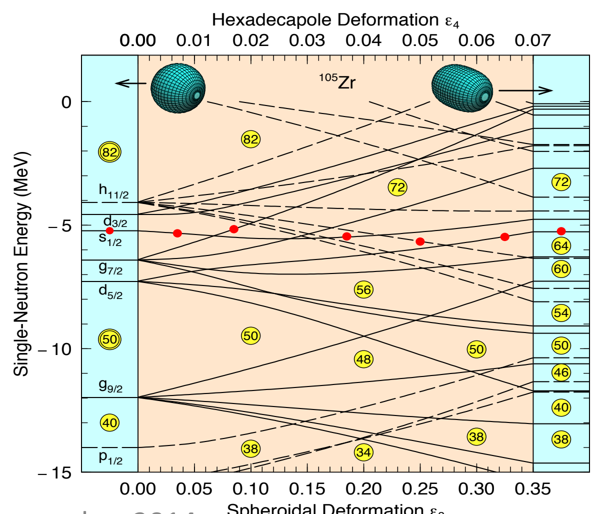
$$\left[-\frac{\hbar^2}{2m}\Delta + V^{\mathrm{n,p}}(\boldsymbol{r})\right]\psi_\nu^{\mathrm{n,p}}(\boldsymbol{r}) = \epsilon_\nu^{\mathrm{n,p}}\,\psi_\nu^{\mathrm{n,p}}(\boldsymbol{r})$$

Solve the Schrödinger equation for neutrons and protons to get the single-particle energies $\{\varepsilon_\nu\}$



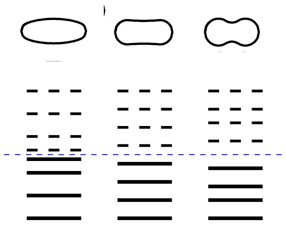
"Nilsson diagrams"





From H. Schatz *et al*, Nature 505 (2014) 62

Nuclear potential energy: shell correction



Single-particle levels in the effective field

Given the neutron or proton levels $\{\varepsilon_\nu\}$

$\delta E = \Sigma_\nu \, \varepsilon_\nu \, \delta n_\nu$

The actual density of states is discrete: $g_0(\varepsilon) = \Sigma_\nu \, g_\nu \, \delta(\varepsilon - \varepsilon_\nu)$

A smooth density of states $\tilde{g}(\varepsilon)$ obtained by convolution: $\tilde{g} = \xi_\gamma * g_0$

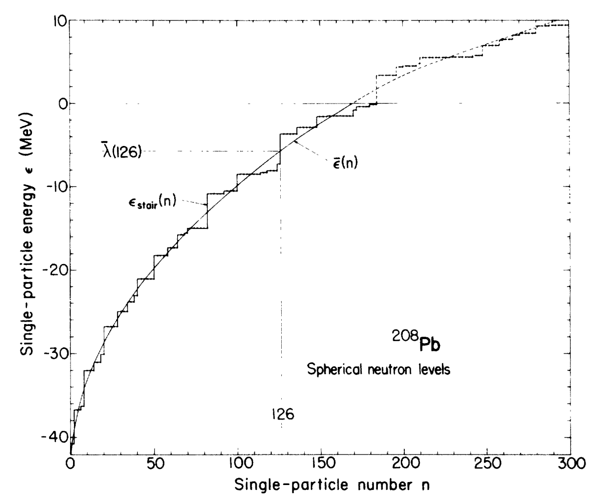
Fermi energy λ: $\int_{-\infty}^{\lambda} \tilde{g}(\epsilon) d\epsilon \doteq N \text{ or } Z$

Shell correction: $\delta E_{\rm shell} = \int_{-\infty}^{\lambda} g_0(\epsilon)\,\epsilon\, d\epsilon - \int_{-\infty}^{\lambda} \tilde{g}(\epsilon)\,\epsilon\, d\epsilon = \sum_{\epsilon_\nu < \lambda} g_\nu \epsilon_\nu - \int_{-\infty}^{\lambda} \tilde{g}(\epsilon)\,\epsilon\, d\epsilon$

Shell correction = staircase minus smooth

Myers & Swiatecki, Nucl Phys 81 (1966) 1

V.M. Strutinsky, Nucl Phys A95 (1967) 420



Nuclear potential energy: pairing correction

BCS: particles are replaced by quasi-particles

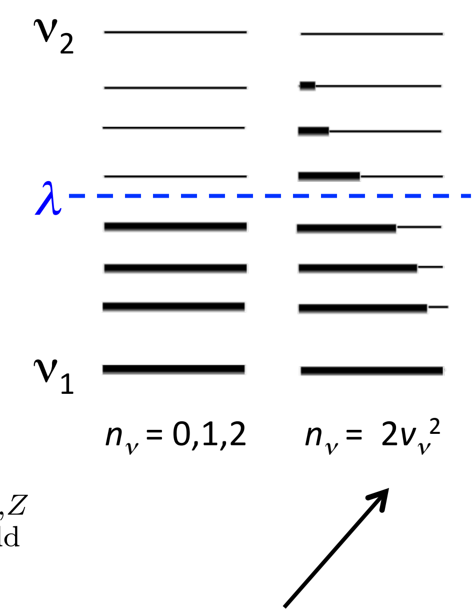
Quasi-particle energy: $E_\nu = \left[(\epsilon_\nu - \lambda)^2 + \Delta^2\right]^{1/2}$

Fermi level λ

Pairing gap Δ

$$N \text{ or } Z \doteq 2(\nu_1 - 1) + 2\sum_{\nu=\nu_1}^{\nu_2} v_\nu^2$$

$$\frac{2}{G} \doteq \sum_\nu \frac{1}{E_\nu} \qquad (g_n=2)$$

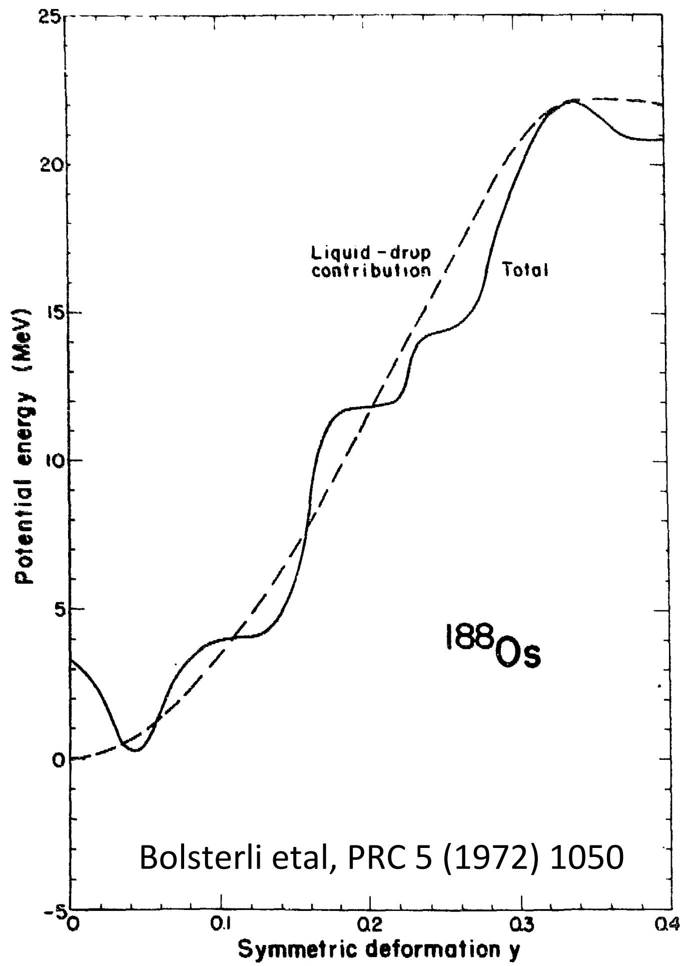


$$v_\nu^2 = \tfrac{1}{2}\left[1 - (\epsilon_\nu - \lambda)/E_\nu\right]$$

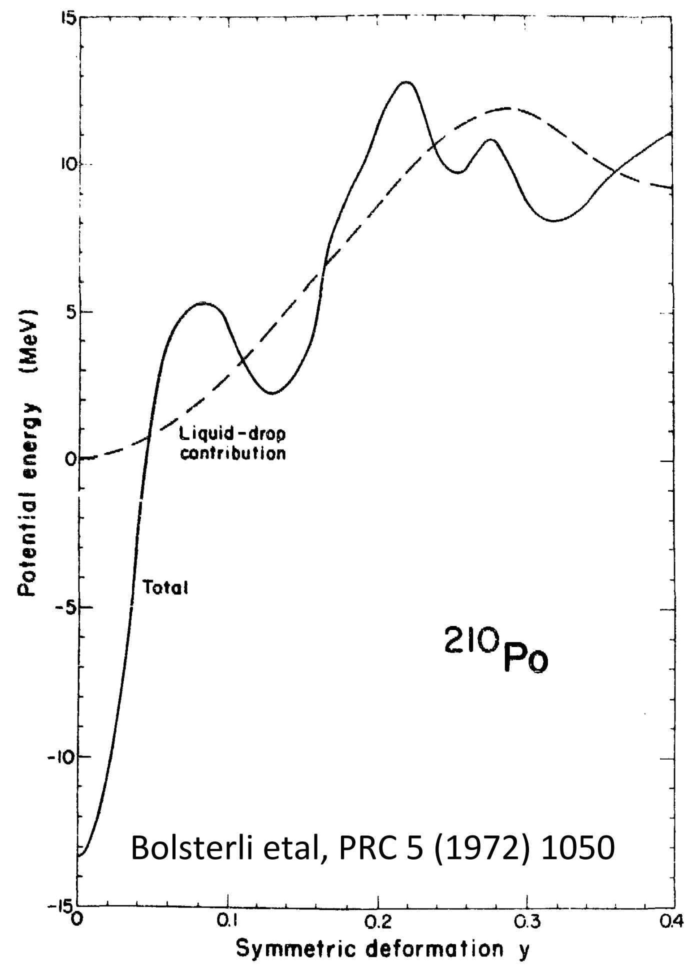
g_0: $$E_{\text{pair}} = \sum_\nu [2v_\nu^2 - n_\nu]\,\epsilon_\nu - \frac{\Delta^2}{G} - \tfrac{1}{2}G\sum_{\nu=\nu_1}^{\nu_2}[2v_\nu^4 - n_\nu] + E_\nu\,\theta_{\text{odd}}^{N,Z}$$

$$\delta E_{\text{pair}} = E_{\text{pair}}[g_0] - E_{\text{pair}}[\tilde{g}]$$

Nuclear potential energy of deformation

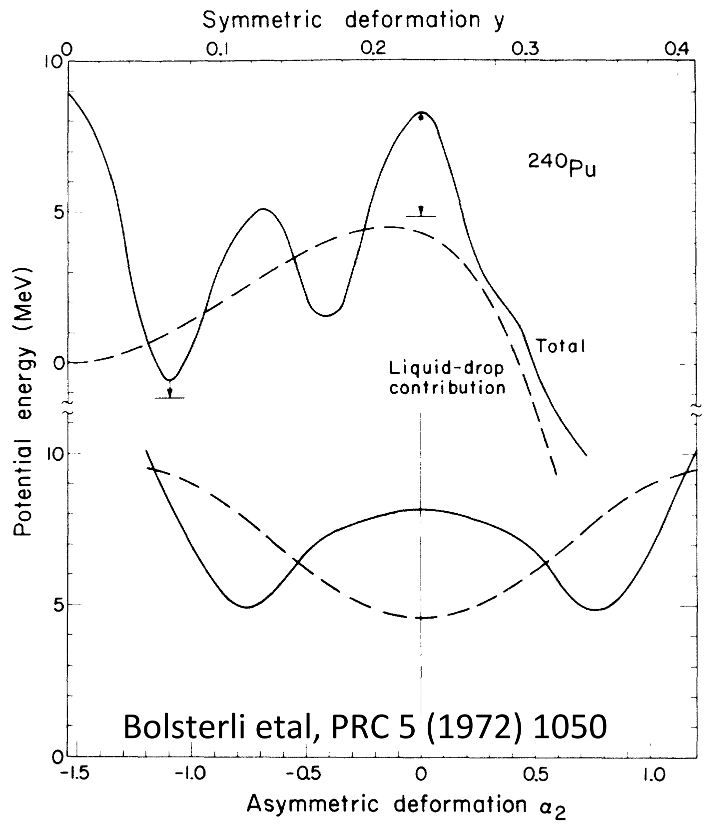


Bolsterli etal, PRC 5 (1972) 1050

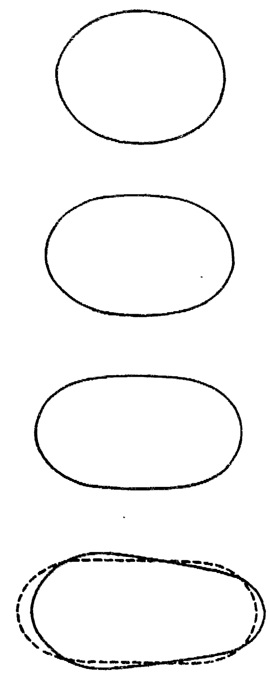


Bolsterli etal, PRC 5 (1972) 1050

Nuclear potential energy of deformation



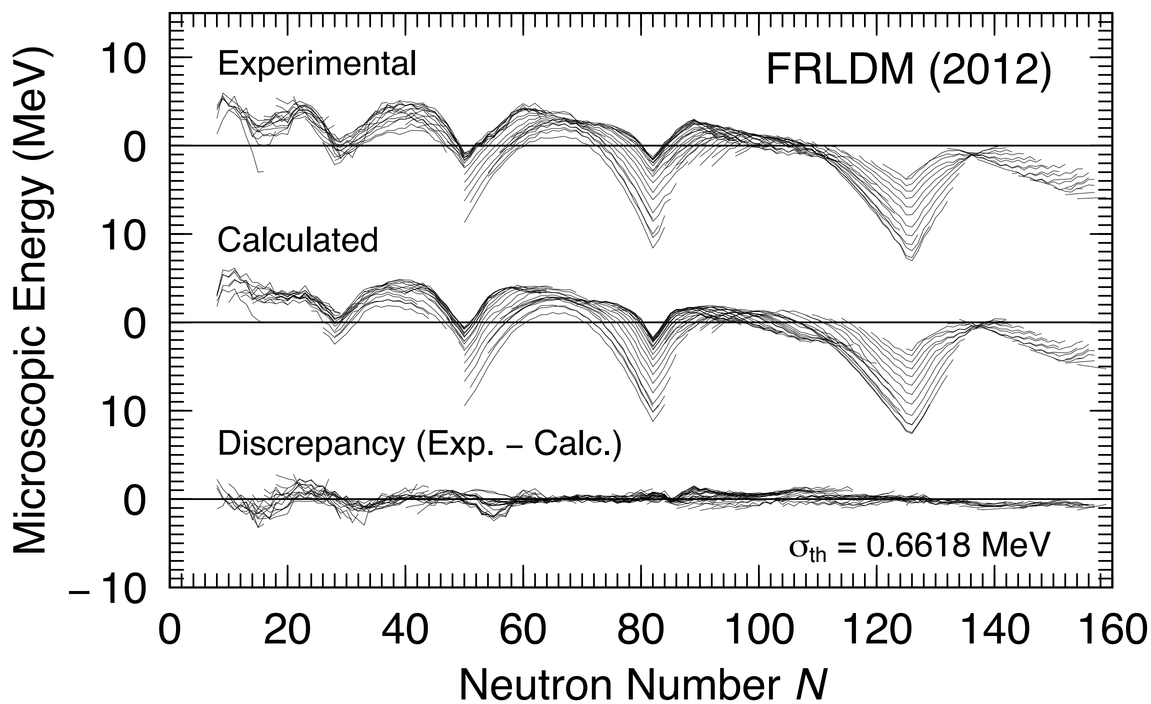
Bolsterli etal, PRC 5 (1972) 1050



Nuclear potential energy: ground-state masses

$$M(Z,N) = E_{macro}(Z,N,\text{g.s.}) + E_{s+p}(Z,N,\text{g.s.})$$

$$= E_{macro}(Z,N,\bigcirc) + E_{micro}(Z,N,\text{g.s.})$$



Nuclear potential energy surfaces

P. Möller, Nucl Phys A 192 (1972) 529:

$E_{macro}(Z,A,\text{shape}) = a_s(1 - \kappa_s^2)A^{2/3} B_1(\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5) + c_1 Z^2/A^{1/3} B_3(\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5) + \ldots$

$E_{s+p}(Z,A,\text{shape})$: Modified-oscillator single-particle potential $V(\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5)$

4D calculation $(\varepsilon_2,\varepsilon_3,\varepsilon_4,\varepsilon_5)$ -> 2D landscape (ε_2 & ε_4, ε_3 & ε_5)

^{236}U: top view

Elongation (ε_2 & ε_4)

Asymmetry (ε_3 & ε_5)

^{236}U: side view

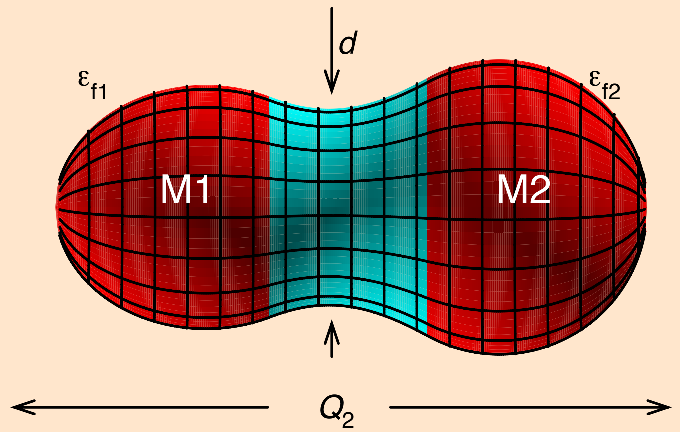
Elongation (ε_2 & ε_4)

P. Möller, Nucl Phys 192 (1972) 529

Nuclear potential energy: 5D shape lattice

Five Essential Fission Shape Coordinates

3QS shape family



I	45	Q_2 ~	Elongation (fission direction)
	⊗		
J	15	d ~	Neck
	⊗		
K	15	ε_{f1} ~	Left fragment deformation
	⊗		
L	15	ε_{f2} ~	Right fragment deformation
	⊗		
M	35	α_g ~	(M1-M2)/(M1+M2) Mass asymmetry

⇒ 5 315 625 grid points – 306 300 unphysical points

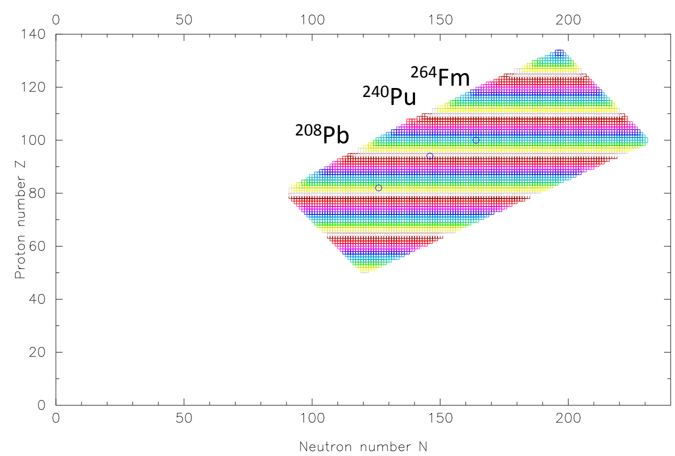
⇒ 5 009 325 physical grid points

P. Möller 2009:

5*D* table of the potential energy

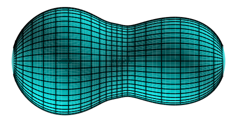
$\{U_{IJKLM}\}$

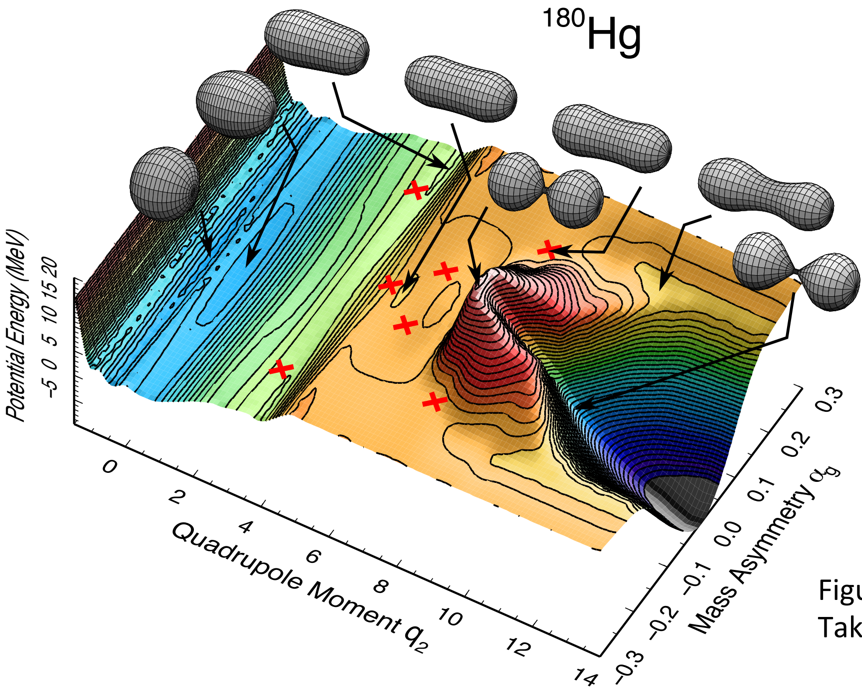
for 5,254 nuclei

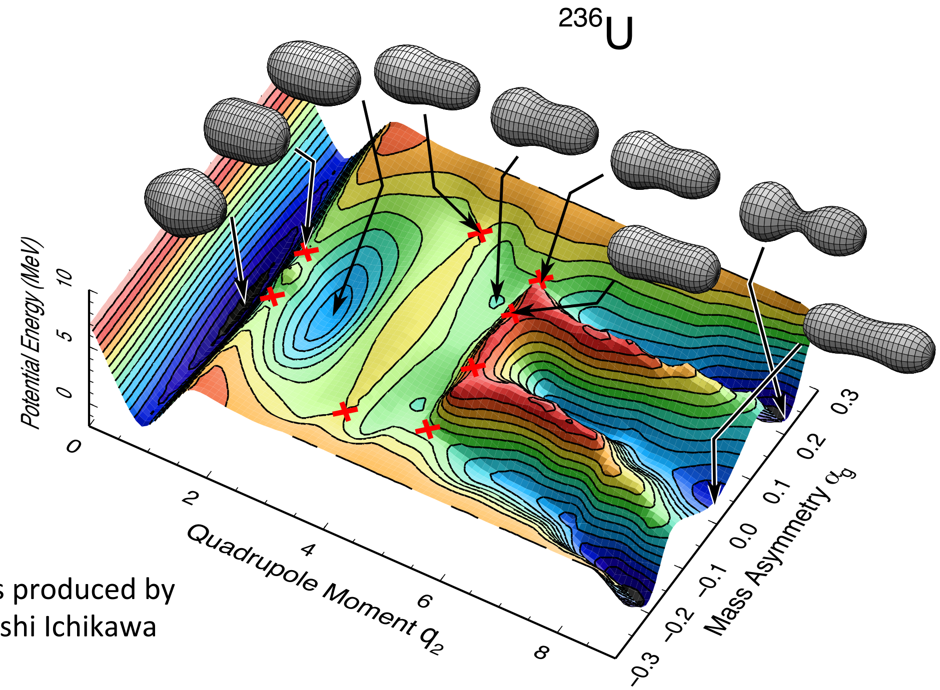


Nuclear potential energy: fission barrier landscape

5D potential-energy surfaces reduced to two dimensions



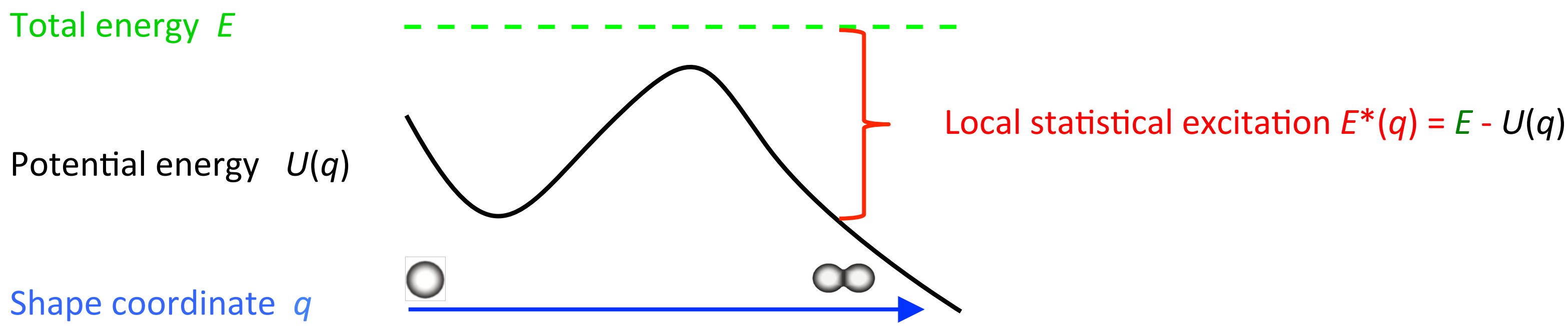




Figures produced by
Takatoshi Ichikawa

Fission dynamics: Temperature

The statistical excitation E^* depends on the shape:



=> Local temperature $T(q)$: $E^* \approx aT^2$

The shell and pairing corrections were calculated for T=0;
they generally decrease with increasing temperature

=> Energy-dependent effective potential energy:

$$U_E(q) = E_{\text{macro}}(q) + E_{\text{s+p}}(q) \times S(E^*(q))$$

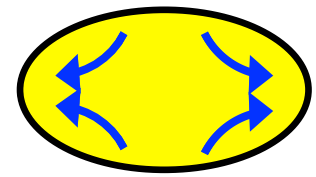
suppression function

J. Randrup and P. Möller,
Phys Rev C 88 (2013) 064606

Inertial mass tensor for nuclear shape motion

Kinetic energy associated with shape changes: $K(\dot{\boldsymbol{q}},\boldsymbol{q}) \;=\; \frac{1}{2}\dot{\boldsymbol{q}}\cdot\boldsymbol{M}(\boldsymbol{q})\cdot\dot{\boldsymbol{q}} \;=\; \frac{1}{2}\sum_{ij}\dot{q}_i\,M_{ij}(\boldsymbol{q})\,\dot{q}_j$

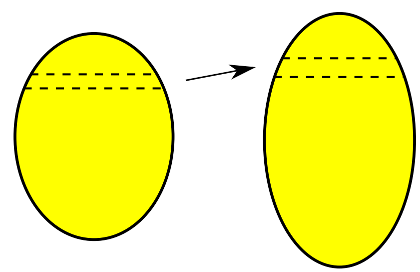
Macroscopic fluid: $K[\rho(\boldsymbol{r}),\boldsymbol{v}(\boldsymbol{r})] \;=\; \frac{1}{2}m\int\rho(\boldsymbol{r})\,\boldsymbol{v}(\boldsymbol{r})^2 d^3\boldsymbol{r}$



The nuclear fluid is incompressible => density is constant: $\rho(\boldsymbol{r}) = \rho_0$

Assume irrotational flow => $\boldsymbol{v}(\boldsymbol{r})$ depends only on shape change

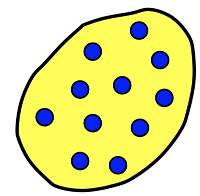
Werner-Wheeler approximation:
the mass within a slice remains
in that slice as the shape changes.



=> $\boldsymbol{M}(\boldsymbol{q})$

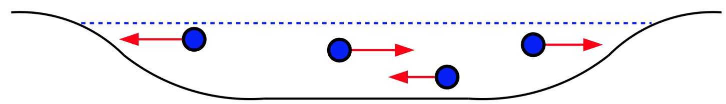
Dissipation for nuclear shape motion: one-body

Individual nucleons move in common one-body mean field
(while occasionally experiencing Pauli-suppressed collisions)



$$h[f](\boldsymbol{r},\boldsymbol{p}) = \frac{p^2}{2m^*} + U[\rho](\boldsymbol{r})$$

Single-particle Hamiltonian



Nucleons in mean field

One-body dissipation:

Density $\rho(\boldsymbol{r})$ changes => mean field changes => nucleons adjust quickly

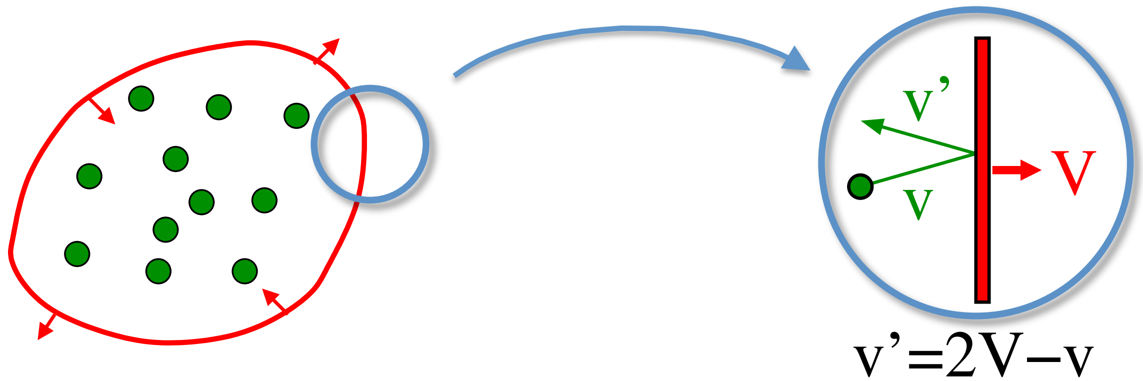
The interaction between the individual nucleon and the residual system is concentrated in the *surface* region: *Fermi gas in a deforming container*

One-body dissipation in a mononucleus:

Wall formula for the dissipation rate

Slowly deforming nucleus:

Nuclei are leptodermous



Dissipation rate: $$\dot{Q}^{\mathrm{wall}}(\boldsymbol{q},\dot{\boldsymbol{q}}) \;=\; m\rho_0\bar{v}\oint V^2 d^2\sigma \;=\; \sum_{ij}\dot{q}_i\gamma_{ij}^{\mathrm{wall}}(\boldsymbol{q})\dot{q}_j \;,$$

Dissipation tensor: $$\gamma_{ij}^{\mathrm{wall}}(\boldsymbol{q}) = 2\pi m\rho_0\bar{v}\int_{z_{\min}}^{z_{\max}}(\rho\frac{\partial\rho}{\partial q_i})(\rho\frac{\partial\rho}{\partial q_j})\left[\rho^2+(\rho\frac{\partial\rho}{\partial z})^2\right]^{-\frac{1}{2}}dz$$

ρ(*z*):

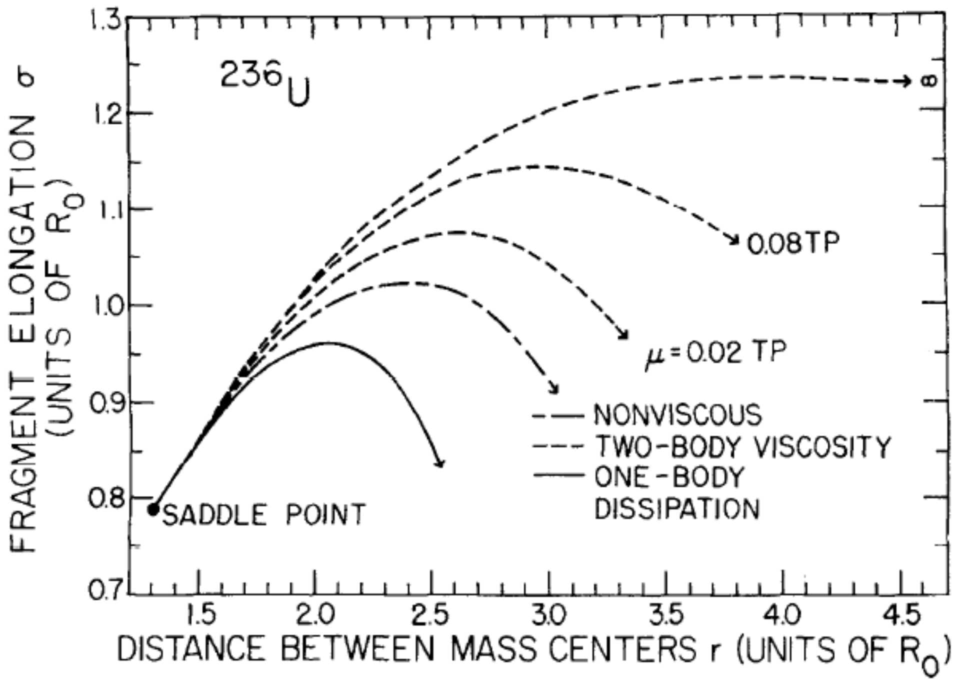
J. Blocki, Y. Boneh, J. R. Nix, J. Randrup, M. Robel, A. J. Sierk, and W. J. Swiatecki, Ann Phys **113** (1978) 330: *One-Body Dissipation and the Super-Viscidity of Nuclei*

Fission dynamics with 1-body & 2-body dissipation

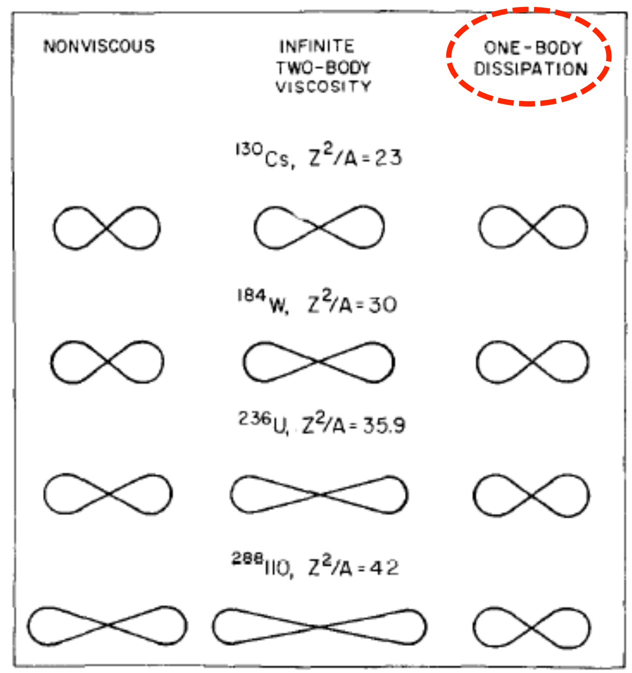
One-body wall formula: $\dot{Q} = \rho \bar{v} \oint V^2 d\sigma$

Strong & E* indep

Shape dynamics from saddle to scission:



Scission shapes:



J. Blocki, Y. Boneh, J. R. Nix, J. Randrup, M. Robel, A. J. Sierk, and W. J. Swiatecki,
Ann Phys **113** (1978) 330: *One-Body Dissipation and the Super-Viscidity of Nuclei*

Fission fragment kinetic energy

J. Blocki, Y. Boneh, J. R. Nix, J. Randrup, M. Robel, A. J. Sierk, and W. J. Swiatecki,
Ann Phys **113** (1978) 330: *One-Body Dissipation and the Super-Viscidity of Nuclei*

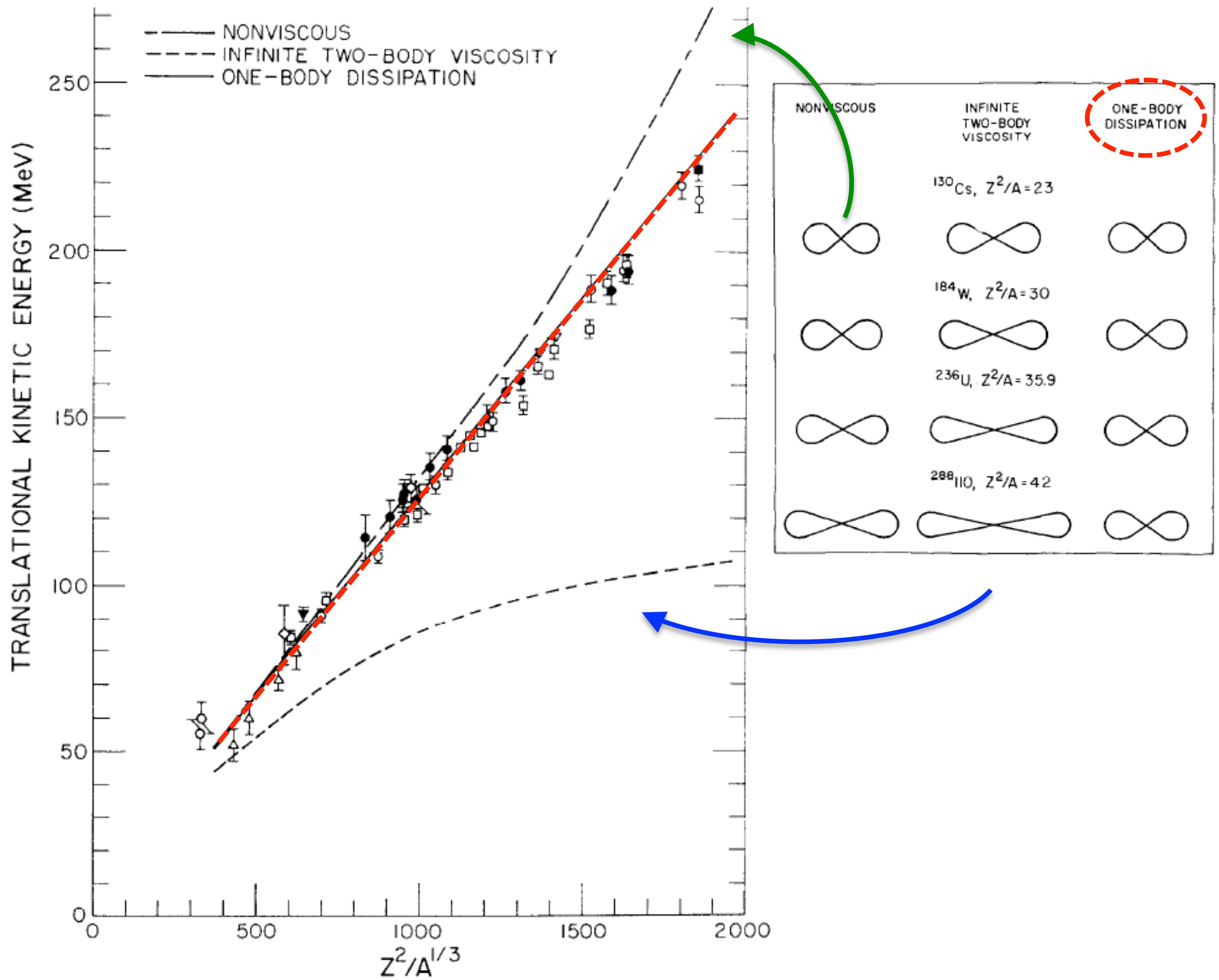
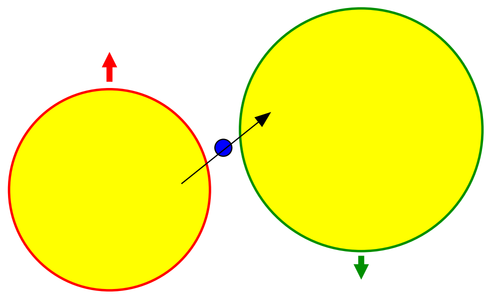


FIG. 6. Comparison of calculated and experimental most probable fission-fragment kinetic energies as a function of $Z^2/A^{1/3}$. The kinetic energies calculated for nonviscous flow are given by the dot–dashed curve. The dashed curve shows the results for infinite two-body viscosity, and the solid curve shows the results for the one-body dissipation considered here. The experimental data are for cases in which the most probable mass division is into two equal fragments; the open symbols represent values for equal mass divisions only and the solid symbols represent values averaged over all mass divisions. The original sources for the experimental data are given in [18].

One-body dissipation in the dinucleus:
Nucleon exchange in damped reactions



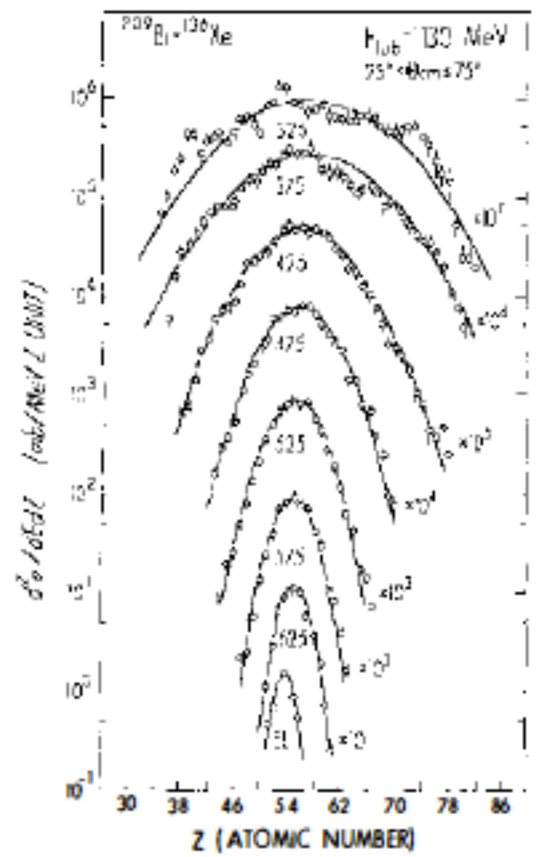
$$Q \sim V_{AB} v_F \mathcal{N}$$

$$Q = -\Delta E_{\rm rel} \qquad \mathcal{N} = \sigma_A^2$$

Dissipated energy

Nucleons exchanged

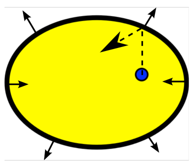
J. Randrup, Nucl Phys A307 (1978) 319; A327 (1979) 490



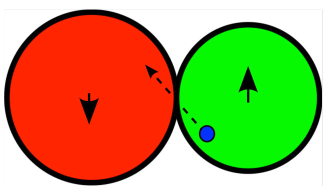
W.U. Schröder & J.R. Huizenga, Ann Rev Nucl Sci 27, 465 (1977)

One-body dissipation in fission:

Wall-plus-window formula



$$\dot{Q}^{\rm wall}(\boldsymbol{q},\dot{\boldsymbol{q}}) \;=\; m\rho_0\bar{v}\oint \dot{n}^2 d^2\sigma \;=\; \sum_{ij}\dot{q}_i\gamma_{ij}^{\rm wall}(\boldsymbol{q})\dot{q}_j$$



$$\dot{Q}^{\rm window} \;=\; \tfrac{1}{4}m\rho_0\bar{v}\,\pi c^2\,(2U_\parallel^2+U_\perp^2) \;=\; \sum_{ij}\dot{q}_i\gamma_{ij}^{\rm window}(\boldsymbol{q})\dot{q}_j$$

$\rho(z)$:

$$\gamma_{ij}^{\rm w+w}(\boldsymbol{q}) \;\equiv\; \gamma_{ij}^{\rm wall}(\boldsymbol{q})+\gamma_{ij}^{\rm window}(\boldsymbol{q}) \;=\; \tfrac{1}{2}m\rho_0\bar{v}\left\{\frac{\partial R}{\partial q_i}\frac{\partial R}{\partial q_j}\pi c^2 \right.$$
$$\left. +\;\pi\int_{z_0}^{z_3}dz\left(\frac{\partial\rho^2}{\partial q_i}-\frac{1}{2}\frac{\partial\rho^2}{\partial z}\frac{\partial R}{\partial q_i}\right)\left(\frac{\partial\rho^2}{\partial q_j}-\frac{1}{2}\frac{\partial\rho^2}{\partial z}\frac{\partial R}{\partial q_j}\right)\left[\rho^2+\frac{1}{4}\left(\frac{\partial\rho^2}{\partial z}\right)^2\right]^{-\frac{1}{2}}\right\}$$

A.J. Sierk & J.R. Nix, Phys Rev C 21 (1980) 982

Nuclear shape dynamics

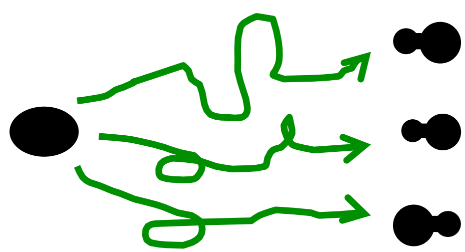
✔ 1) Parametrized family of nuclear shapes: $\boldsymbol{q} = \{q_i\}$  3QS

✔ 2) Potential energy of deformation: $U(\boldsymbol{q}) = U(q_1, q_2, \ldots)$ $U_{\mathrm{macro}} + U_{s+\mathrm{p}}$

✔ 3) Inertial mass tensor: $\boldsymbol{M}(\boldsymbol{q}) = \{M_{\mathrm{ij}}(\boldsymbol{q})\}$ Werner-Wheeler

✔ 4) Dissipation tensor: $\gamma(\boldsymbol{q}) = \{\gamma_{\mathrm{ij}}(\boldsymbol{q})\}$ Wall + Window

Langevin equation of motion: $d\boldsymbol{p}/dt = \boldsymbol{F}^{cons} + \boldsymbol{F}^{diss}$



Fission dynamics: Formal framework

Lagrangian: $$\mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}}) \;=\; \tfrac{1}{2}\sum_{i,j}^{N}\dot{q}_i M_{ij}(\boldsymbol{q})\,\dot{q}_j - U(\boldsymbol{q})$$

Momentum: $$p_i(\boldsymbol{q},\dot{\boldsymbol{q}}) \;=\; \frac{\partial}{\partial\dot{q}_i}\mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}}) \;=\; \sum_j M_{ij}(\boldsymbol{q})\,\dot{q}_j$$

Conservative dynamics: $$\frac{\partial}{\partial t}p_i \;\doteq\; \frac{\partial}{\partial q_i}\mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}}) \;=\; \tfrac{1}{2}\sum_{jk}\dot{q}_j\dot{q}_k\frac{\partial}{\partial q_i}M_{jk}(\boldsymbol{q}) - \frac{\partial}{\partial q_i}U(\boldsymbol{q})$$

Conservative force: $\boldsymbol{F}^{cons} = \boldsymbol{F}^{mass} + \boldsymbol{F}^{pot}$

Dissipative force: $\boldsymbol{F}^{diss} = \boldsymbol{F}^{fric} + \boldsymbol{F}^{ran}$

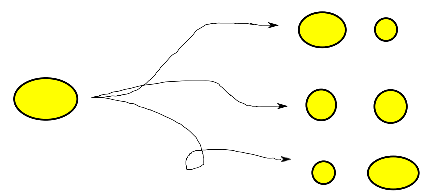
Friction force: $$F_i^{\rm fric}(\boldsymbol{q},\dot{\boldsymbol{q}}) = \langle F_i^{\rm diss}(\boldsymbol{q},\dot{\boldsymbol{q}})\rangle = -\sum_j \gamma_{ij}(\boldsymbol{q})\,\dot{q}_j$$

Random force: $$\langle F_i^{\rm ran}(\boldsymbol{q},t)F_j^{\rm ran}(\boldsymbol{q},t')\rangle = 2\gamma_{ij}(\boldsymbol{q})\,T\,\delta(t-t')$$

Both are prop to γ:
Fluct-Diss Theorem
(Einstein Relation)

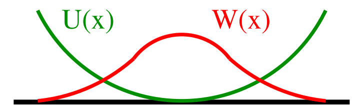
Dissipative dynamics: $$\dot{\boldsymbol{p}} \;=\; \boldsymbol{F}^{\rm cons} + \boldsymbol{F}^{\rm diss}$$

Langevin equation



Langevin dynamics: Equilibration

One dimension, constant m, γ, T,
harmonic potential $U(x) = ½kx^2$:



=> Ensemble: $\{x(t),p(t)\}$

1st and 2nd moments:

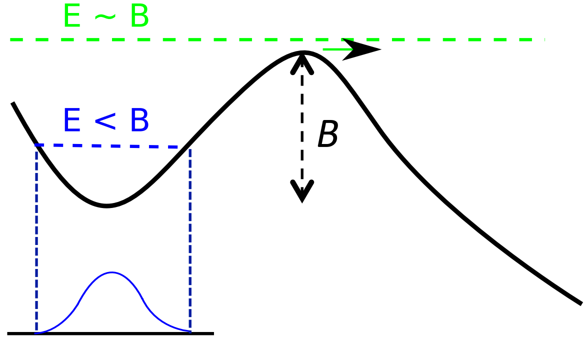
t -> ∞:

$<x(t)>$ -> 0 $\quad$ $<p(t)>$ -> 0

$<x(t)^2>$ -> T/k $\quad$ $<p(t)^2>$ -> mT

Distribution function $W(p,q,t)$:

-> $exp(-p^2/2mT - kx^2/2T) = e^{-E/T}$



$E < B$: Quasi-equilibrium is established,
slow leakage over the barrier

$E < B$: Equilibrium is established

Strongly damped nuclear shape dynamics: Brownian motion

Dissipation is *strong* => Creeping evolution => Acceleration and $(\text{velocity})^2$ are small => Inertial mass is unimportant

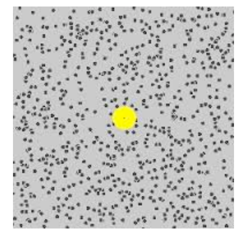
Langevin equation → *Smoluchowski equation*

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

driving force ($\boldsymbol{F}^{\rm pot}$)

dissipative force ($\boldsymbol{F}^{\rm fric} + \boldsymbol{F}^{\rm ran}$)

$F^{\rm fric} = -\gamma \bullet d\chi/dt$



Brownian motion

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

Mobility tensor:

$$\boldsymbol{\mu}(\boldsymbol{\chi}) \equiv \boldsymbol{\gamma}(\boldsymbol{\chi})^{-1}$$

Easy to simulate:

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

mobility eigenvector ($\tilde{\chi}_i^{(n)}$, $\tilde{\boldsymbol{\chi}}^{(n)}$)

random number (ξ_n): $<\xi_n> = 0$, $<\xi_n^2> = 1$

Strongly damped nuclear shape dynamics: Metropolis walk

Dissipation is *strong* => Creeping evolution => Acceleration and (velocity)^2 are small => Inertial mass is unimportant

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

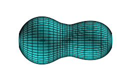
Ignore $M(\chi)$ but still need $U(\chi)$ <u>and</u> $\gamma(\chi)$

Dissipation is *strong* => Large degree of equilibration => Little sensitivity to the structure of γ*?*

If there is indeed only little sensitivity to the structure of the dissipation tensor, then why not try with something simple? For example an *isotropic* tensor:

$$\gamma_{ij}(\boldsymbol{\chi}) = \gamma_0(\boldsymbol{\chi})\,\delta_{ij}$$

If dissipation tensor is isotropic => Metropolis walk on the U_{IJKLM} *lattice*

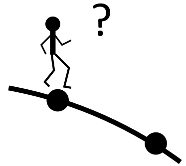


Need <u>only</u> $\{U_{IJKLM}\}$

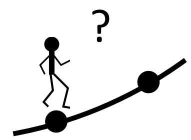
J Randrup & P Möller, Phys Rev Lett 106 (2011) 132503

Metropolis walk …

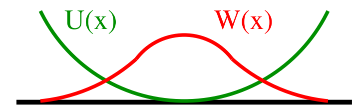
Metropolis *et al.* (1953):



$P_{down} = 1$



$P_{up} = \exp(-\Delta U/T)$



W(x) -> exp(-U(x)/T)

… on the potential-energy surface:

Start at ground-state (or isomeric) minimum

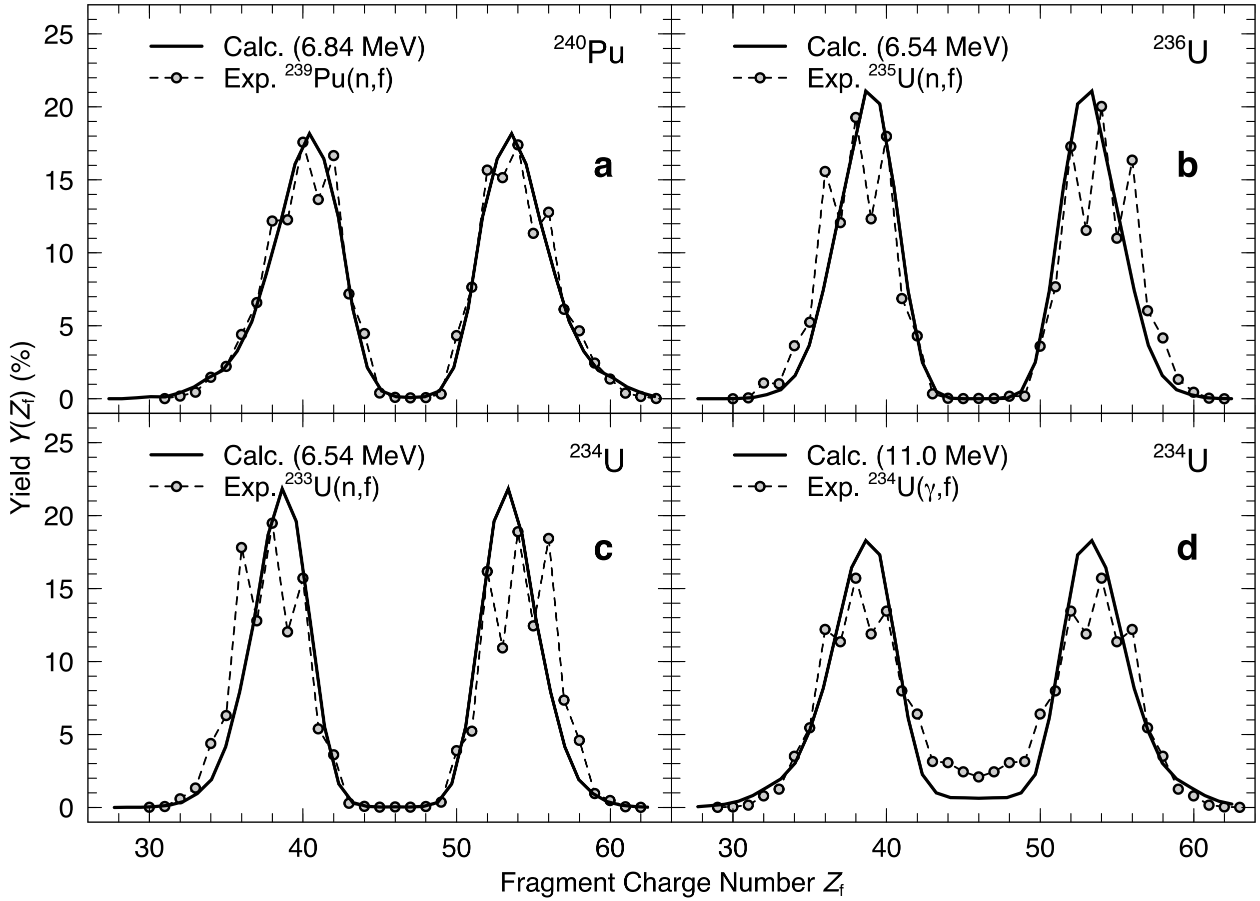
Asymmetry

Walk until the neck has become thin

Elongation →

The very first Metropolis results:

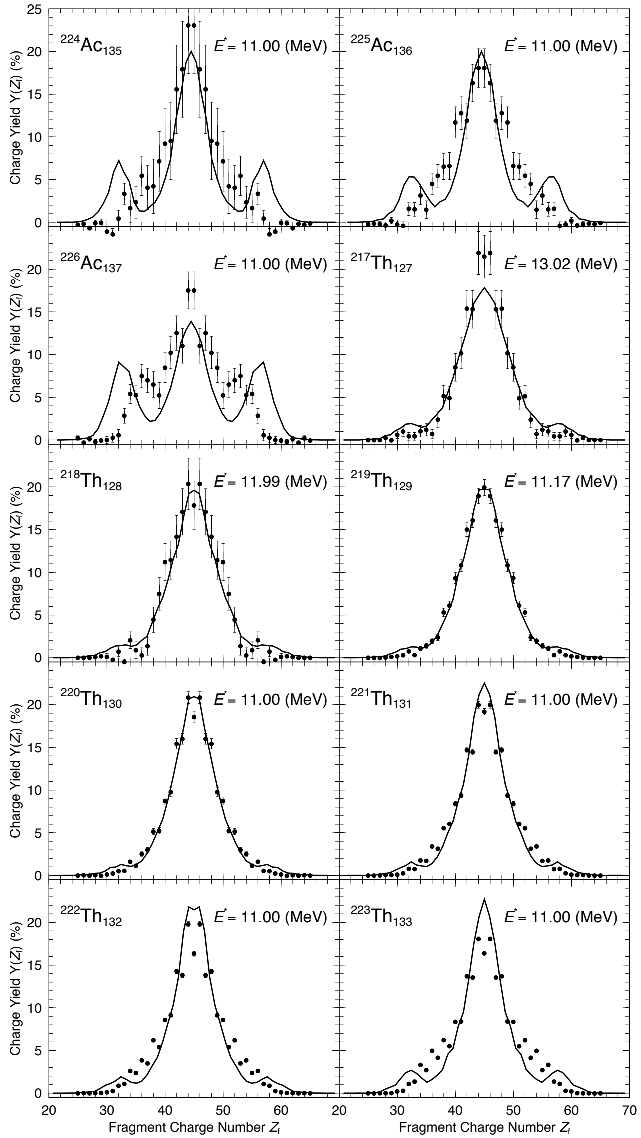
J. Randrup & P. Möller, PRL 106 (2011) 132503



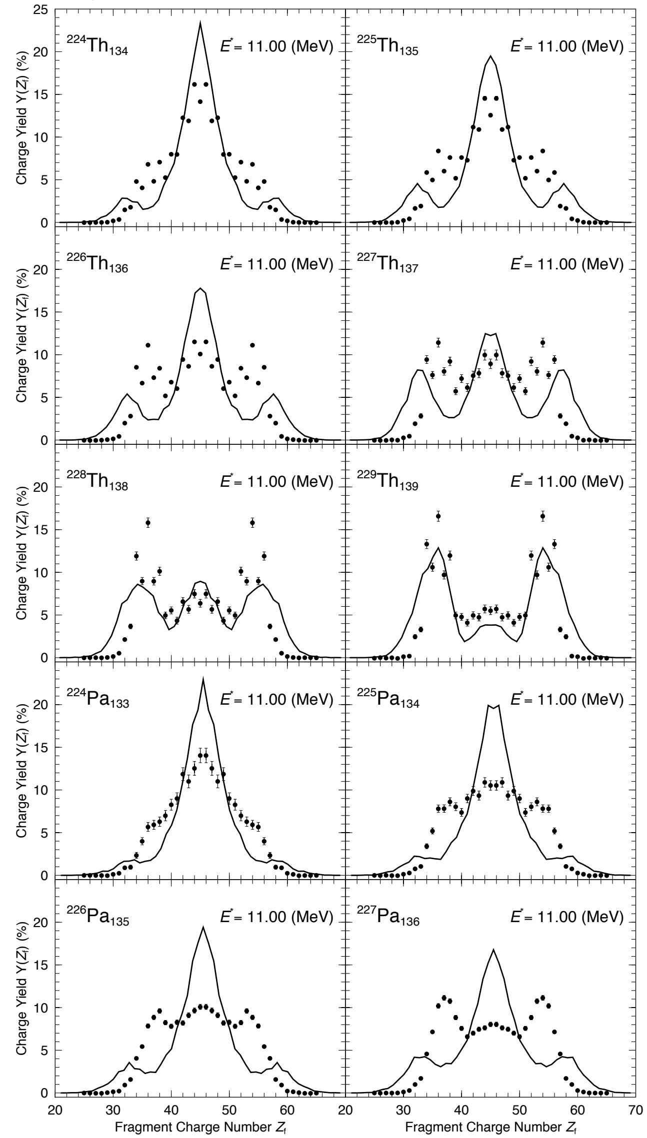
The Metropolis method looks remarkably promising -
let's benchmark it against 70 measured charge yields …

Comparison with data from K.H. Schmidt *et al.*, NPA 665 (2000) 221

$P(Z_f)$ for isotopes at E^*=11 MeV



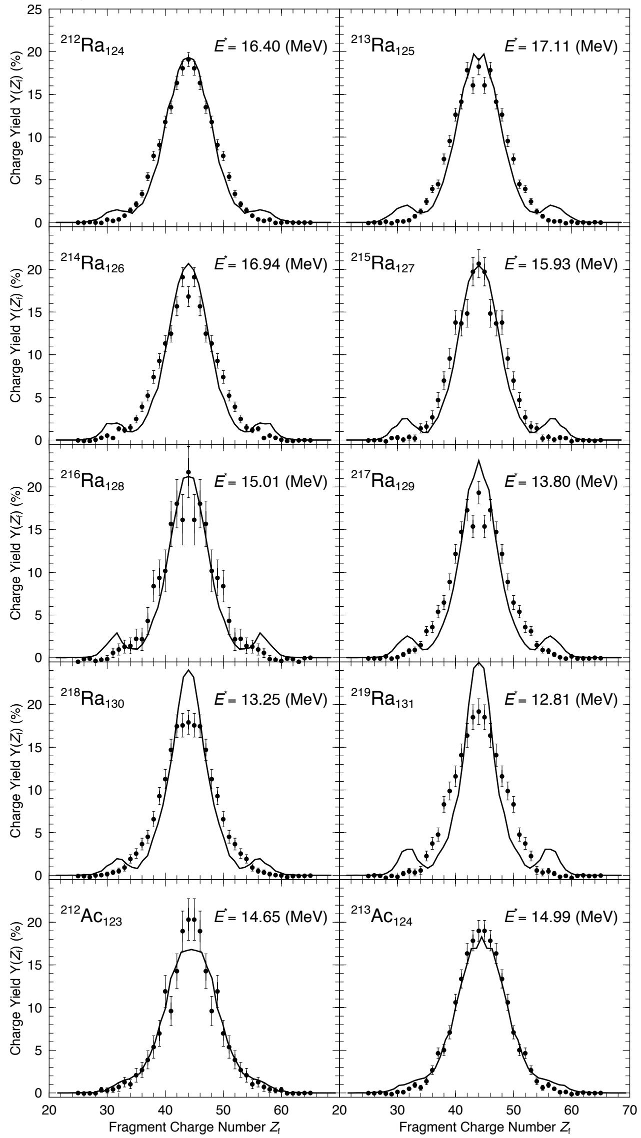
$P(Z_f)$ for isotopes at E^*=11 MeV



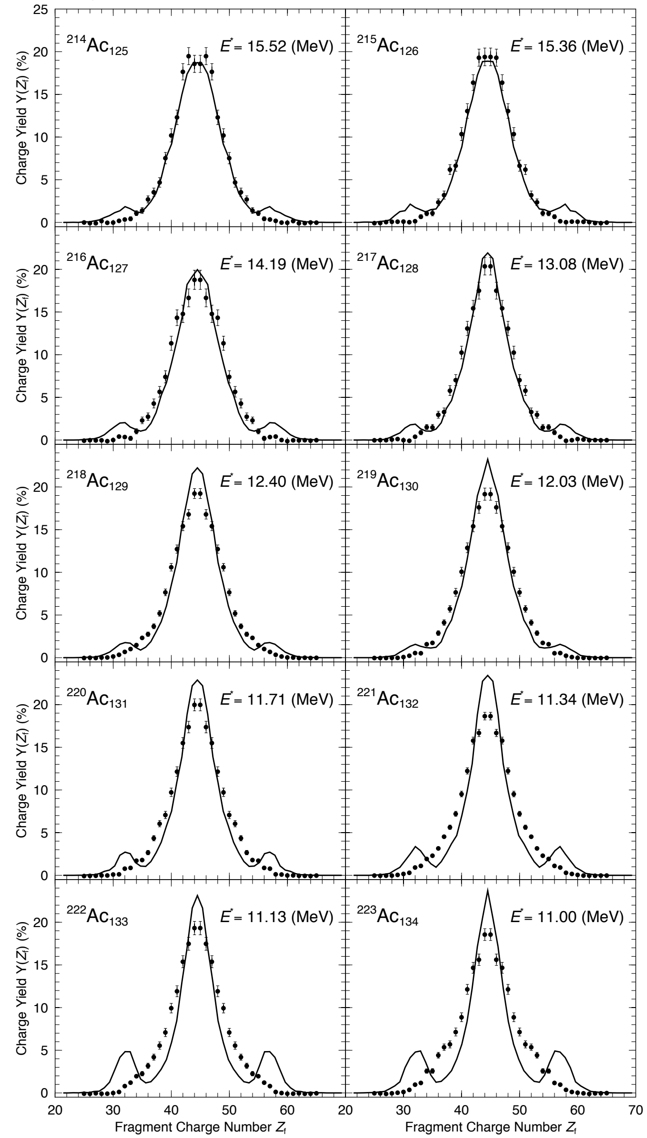
J. Randrup & P. Möller, Phys. Rev. C **88**, 064606 (2013)

Comparison with data from K.H. Schmidt *et al.*, NPA 665 (2000) 221

P(Z_f) for isotopes at E=11 MeV*



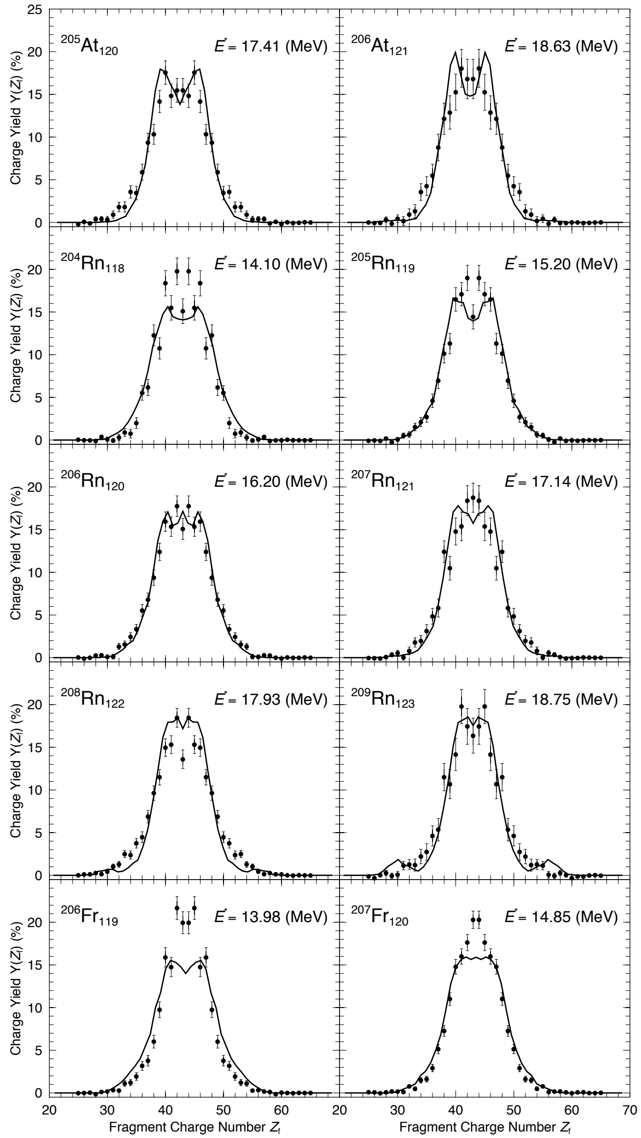
P(Z_f) for isotopes at E=11 MeV*



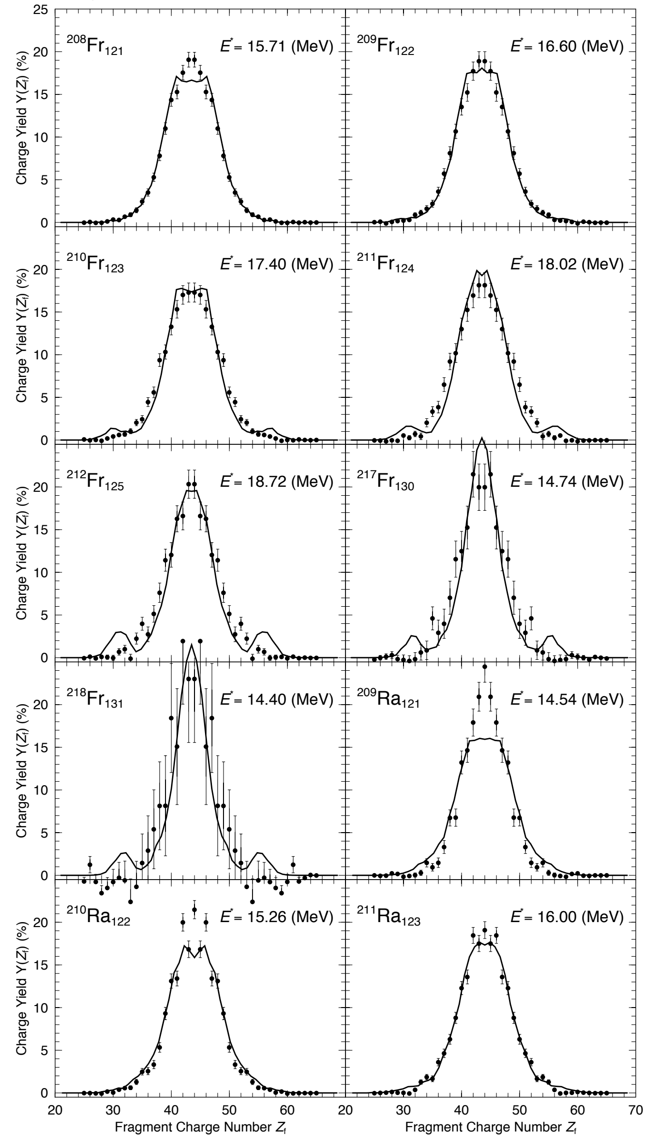
J. Randrup & P. Möller, Phys. Rev. C **88**, 064606 (2013)

Comparison with data from K.H. Schmidt *et al.*, NPA 665 (2000) 221

P(Z_f) for isotopes at E=11 MeV*

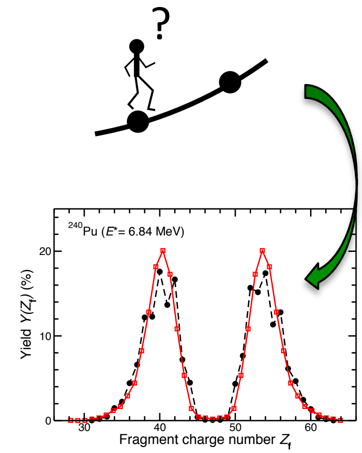


P(Z_f) for isotopes at E=11 MeV*



J. Randrup & P. Möller, Phys. Rev. C **88**, 064606 (2013)

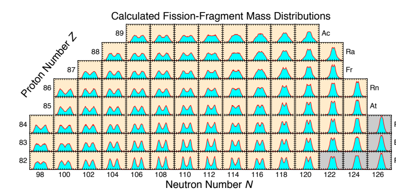
Nuclear shape dynamics: Metropolis?



The Metropolis walk method, used with the tabulated 5D 3QS potential-energy surfaces, provides a powerful tool for calculating fission-fragment mass distributions

Special advantages: *predictive power, ease of computation*

> 5,000 nuclei: $\{U_{IJKLM}\}$ ≈ minutes/10k events

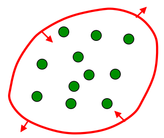


But: *How reliable is it?*

It is based on the assumption that the mass yields are not sensitive to the details of the dissipation

This can be checked:

Solve the Smoluchowski equation with a <u>range</u> of dissipation tensors:
How much are the fragment mass yields affected?



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

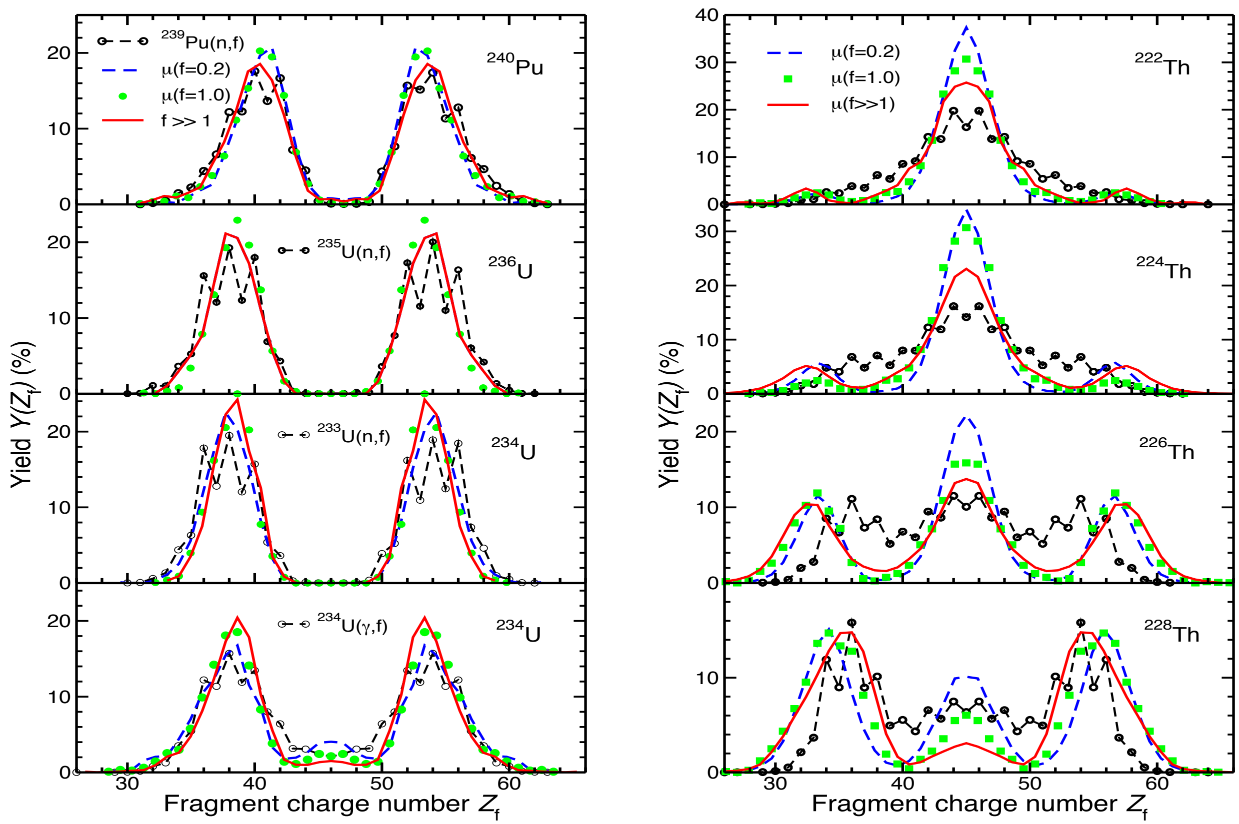
=> $\gamma(\chi)$

Dependence of $P(Z_f)$ on the dissipation tensor

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

Go from wall dissipation to isotropic dissipation:

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

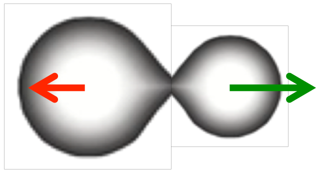


Nuclear shape dynamics: Strongly damped?

How good is the strongly damped idealization?

Probably not good near scission

Cannot provide kinetic energies



The remarkable success of the recent mass-yield calculations (which were based on the strongly damped limit) gives us *hope* that the full Langevin treatment could provide a quantitative means for calculating *both* fragment yields *and* energies

Fission dynamics: Full Langevin simulations

Preliminary results by Arnie Sierk (talk Friday AM)

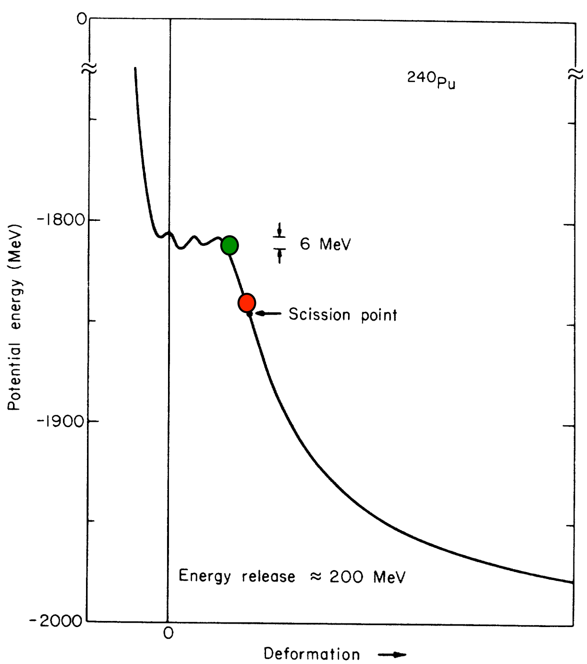
Three-quadratic-surfaces shape family
Macroscopic-microscopic potential
Werner-Wheeler inertial masses
Wall-plus-window one-body dissipation*)

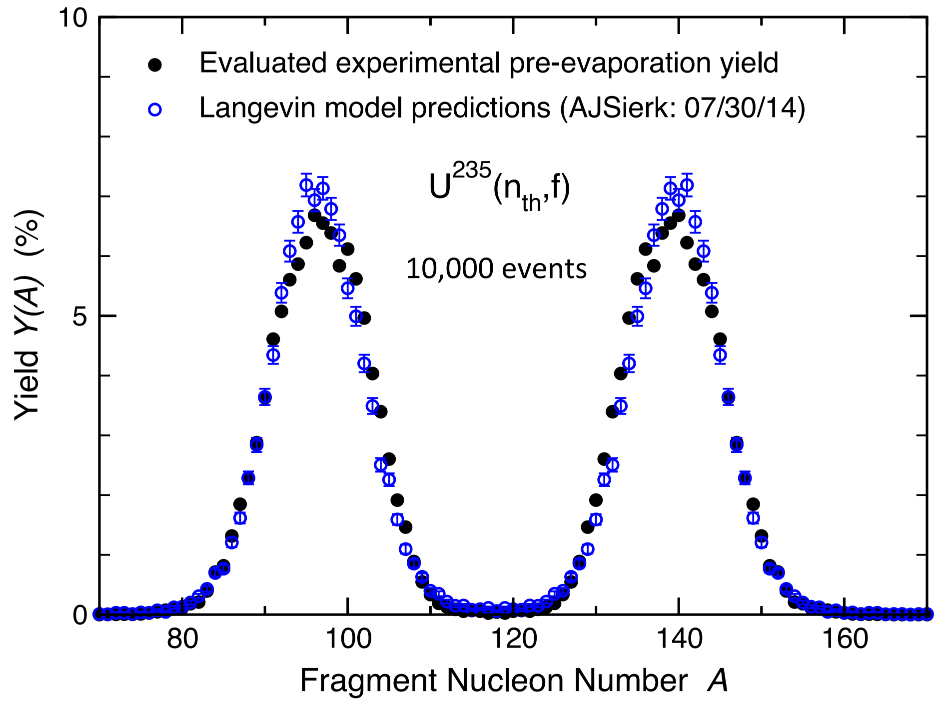
*) with somewhat reduced strength

Start beyond last saddle:
sample $\boldsymbol{q}$ and $d\boldsymbol{q}/dt$

Langevin propagation

Stop before scission:
extract mass partition

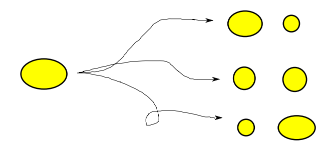




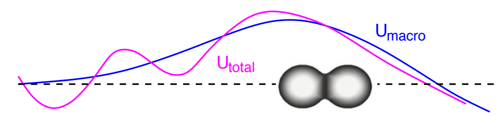
Fission dynamics

within the macroscopic-microscopic approach

Fission dynamics concerns primarily the *dissipative shape evolution*; the *Langevin equation* provides the appropriate formal framework (from a single compound nucleus to an *ensemble* of final configurations)

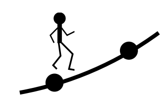


Nuclear *potential energy* surfaces can be fairly reliably calculated with the macroscopic-microscopic method (masses, barriers, …); need: *energy-dependent* surfaces

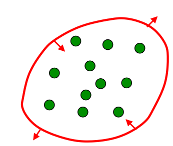


Talk by Peter Möller

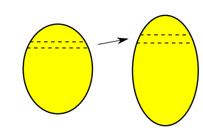
Strongly damped shape dynamics is akin to Brownian motion; the *Metropolis walk* method offers a useful starting point



There is supportive evidence for the dominance of *one-body dissipation*, and the *wall+window formula* (with reduced strength) seems to work well, but it is still purely *macroscopic* (no shell or pairing effects included yet!)



Inertial *masses* are poorly understood, so *macroscopic* inertias are being used in the simulations (but they may be *less crucial?*)



Full *Langevin simulations* are highly desirable; they have recently become feasible (*but* are still slow)

Talk by Arnie Sierk

Fission **E**xperiment**S** and **T**heoretical **A**dvances

Santa Fe, New Mexico, 8-12 September 2014

End of

Lectures on Fission Dynamics
within the Macroscopic-Microscopic Approach

Jørgen Randrup
LBNL, Berkeley, California

BERKELEY LAB
LAWRENCE BERKELEY NATIONAL LABORATORY