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GEMINI: Dexcitation of excited compound nuclei through a series of binary decays

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GEMINI code Robert Charity

Monte Carlo statistical-model code to follow the decay of a compound nucleus by a series sequential binary-decays.

Angular-momentum consistent formalism.

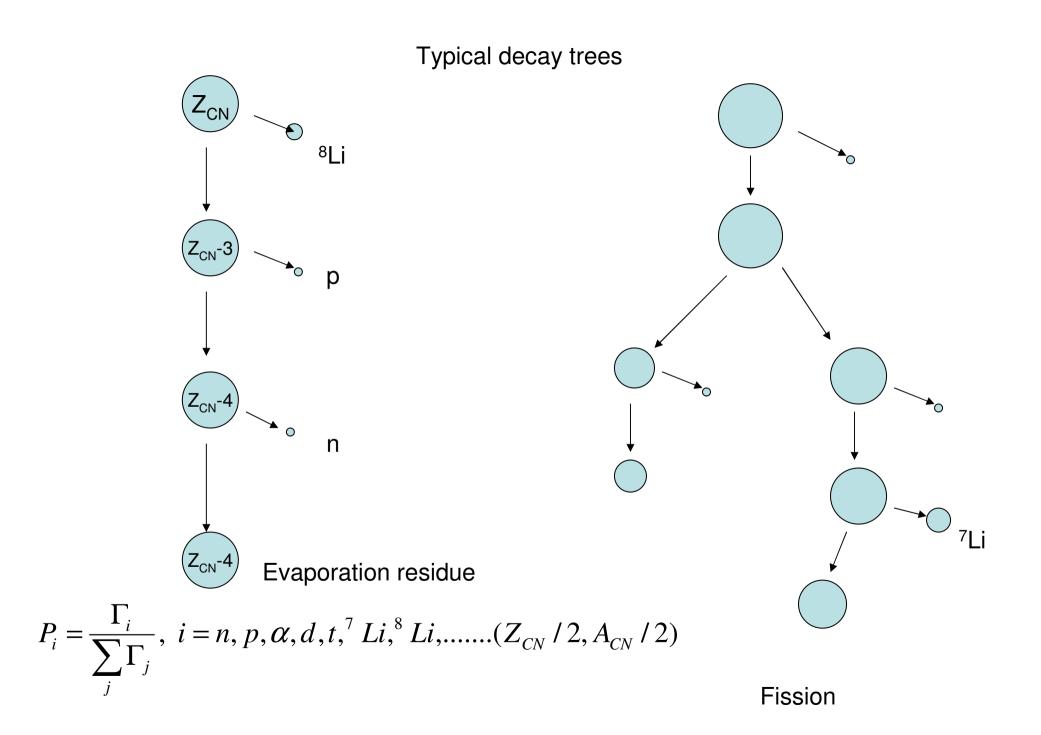




GEMINI

- Born 1986 (Berkeley, Darmstadt, St. Louis)
- Not written to predict, but to interpret data and test sensitivity to different physics.
- Fortran95 (on web) and C++ versions
- Lot of options, user chooses.
- Written for heavy-ion fusion reactions

 a) only equilibrium decay.
 - b) must handle large angular momentum
 - c) E*/A<3MeV.



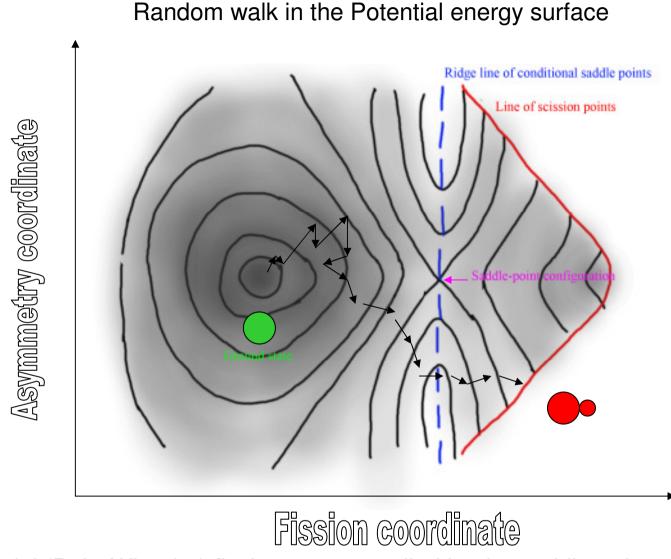
General binary decay mode of a compound nucleus

- Very-asymmetric split– light-particle evaporation (n,p,α,Li,...)
 Weisshopf-Ewing or Hauser-Feshbach formulism
- Symmetric split fission
 Bohr-Wheeler (Transition-state) formalism (1Dim)– needs fission barrier
- Morreto (Nucl. Phys. A247 (1975) 211) considered a generalized binary-decay mode where all asymmetric mass slits were allowed (2Dim)

Includes evaporation and fission as its extremes.

modified transition-state formulism

Requires conditional fission barriers for each asymmetry.



1-d model (Bohr Wheeler) fission rate controlled by the saddle-point energy2-d model (Moretto) asymmetry determined by conditional saddle point.asymmetry not changed in transition from saddle to scission?

GEMINI Details

- Z_imf_min =3,4,5 user parameter
- If (Z < Z_imf_min) Γ(Z,A) from Hauser-Feshbach formalism (n,p,d,t,³He,α,⁶He,⁸He,⁶Li,⁶Li^{*}'s,⁷Li,...¹⁰Be,¹⁰Be^{*}'s) excited states of evaporated particle up to E^{*}=5 MeV
- If $(Z \ge Z_{inf}) \Gamma(Z,A)$ from Moretto's transition-state formalism
- Gamma-decay decay also included.
- Spin and spin orientation of all particles determined needed for angular distributions at large angular momenta. Requires initial orientation.
- Velocities and emission angles of all particle are determined, not always isotropic, but symmetry about 90°.
- Decay cascade followed until a binary decay is not possible.

Light-particle evaporation, n,p,d,t,³He,α,^{6,7,8,9}Li^{*},^{7,8,9,10,11}Be^{*}

Hauser-Feshbach formulism – most appropriate for large angular momenta

$$\Gamma_{i} = \frac{1}{2\pi\rho_{CN}(E^{*}, S_{0})} \int d\varepsilon \sum_{s_{2}=0}^{\infty} \sum_{J=|S_{0}-S_{2}|}^{S_{0}+S_{2}} \sum_{l=|J-S_{1}|}^{J+S_{1}} T_{l}(\varepsilon)\rho(E^{*}-B_{i}-\varepsilon, S_{2})$$

$$T_{l}(\varepsilon) = \text{transmission coef. (related to } \sigma_{\text{inv}})$$

$$\varepsilon, S_{1} = \text{kinetic energy ans spin of evaporated particle}$$

$$S_{2} = \text{spin of daughter}$$

$$B_{i} = \text{separation energy}$$

$$\overrightarrow{S_{0}} = \overrightarrow{S_{2}} + \overrightarrow{S_{1}} + \overrightarrow{l}, \quad \overrightarrow{J} = \overrightarrow{S_{1}} + \overrightarrow{l}$$

Need level densities, transmission coefficients, and separation energies

Separation energies from experimental mass or if unknown from Moller-Nix

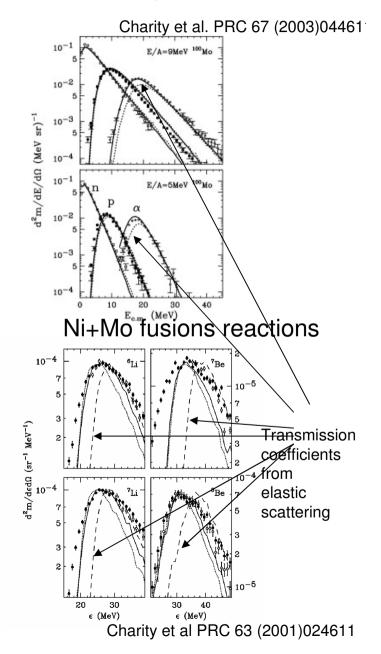
Transmission coefficients

- From global optical-model fits to elasticscattering data (detailed balance => evaporation Coulomb barrier is same as absorption barrier)
- For faster calculation, there is an option

 $T_{I}(\varepsilon) = 0, \ \varepsilon < V_{C}(I)$ $T_{I}(\varepsilon) = 1, \ \varepsilon > V_{C}(I)$

Problem with transmission coefficients for α and heavier particles

- Weiskopf formalism derived from principle of detailed balance – evaporation is the time-reversed equivalent of absorption – this implies that we should be able to can use transmission coefficients obtained from global optical-model fits to elastic scattering data. WRONG
- These Coulomb barriers are too large
- They will underpredict the yield of alpha and heavier fragments
- Increase radius of nuclear potential by 10% for A=170, more for heavier systems (Fineman 1994)–
- will systematize in future.
- With also be important for σ_{inv}

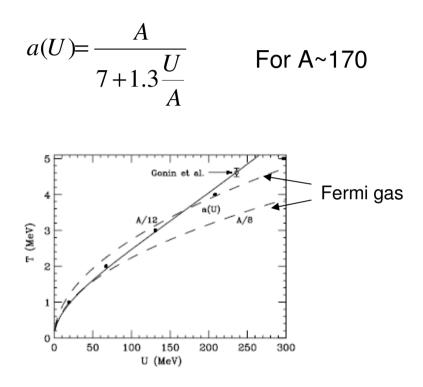


Level Densities

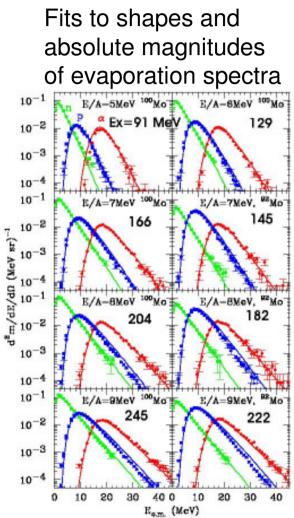
 $\rho(E^*, S) \propto (2S+1) \exp\left[2\sqrt{a(E^*-E_{rot}(S))}\right]$

- Spin dependent Fermi-gas formula
- Backshifted for pairing
- Shell effects fade out according to Ignatyuk
- Many options for level-density parameter "a" (deformation dependent – excitation energy dependent)
- Rotational energies E_{rot} from Finite-Range Liquid-Drop of Sierk
- Collective enhancement and fadeout according to Hansen and Jensen doesn't work.

Excitation-energy dependence of level-density parameter.



Energy-dependent effective mass -> 1.00 Loss of coupling of single-particle degrees of freedom to surface vibrations Increases multiplicity of low-yield particles, Fission mass distributions



Charity et al. PRC 67 (2003)044611

Deviations from Fermi gas behavior seem to increase with increasing mass [Fineman PRC50, 1991 (1994)] Predictions by Shlomo and Natowitz d, t, ³He yields in fusion reactions are always a factor of two lower than statistical model estimates.

In next version of GEMINI this scaling will be incorporated.

Other Binary decays (symmetric and asymmetric fission)

First consider Bohr-Wheeler (transition state) for symmetric fission

$$\Gamma_{BW}^{f} d\varepsilon = \frac{1}{2\pi\rho_{CN}(E^{*},S)} \int \rho[E^{*}-B(S)-\varepsilon,S]d\varepsilon$$

Moretto's original formalism Nucl. Phys. A247 (1975) 211 Thermal distribution along the ridge-line of conditional saddle points

$$\Gamma(y)d\varepsilon \, dy \, dp_{y} = \frac{1}{2\pi\rho_{CN}(E^{*})} \int \rho \left[E^{*} - B(y) - \varepsilon - \frac{p_{y}^{2}}{2m_{y}} \right] d\varepsilon \frac{dydp_{y}}{h}$$

 ε = kinetic energy in fission coordinate

y = asymmetry coordinate

 $p_y = \text{conjugate momenta}$

B(y) =conditional barrier

 m_y = inertia for motion in y coordinate

 $\rho(E^*)$ = level density as function of excitation energy

Integrate over p_v

$$\Gamma d\varepsilon \, dy = \frac{1}{2\pi\rho_{CN}(E^*)} \frac{\sqrt{2\pi T m_y}}{h} \rho [E^* - B(y) - \varepsilon] d\varepsilon \, dy$$

Most important ingredient is the level densities at the conditional saddle points

Conditional barriers

Angular-momentum dependent conditional barriers from Finite-Range Liquid-Drop model (Sierk)– interpolated from full calculations for ¹¹¹In,¹⁴⁹Tb,¹⁹⁴Hg and from a two-spheroid approximation for lighter nuclei. No shell corrections – no doublehumped mass distributions.

B(Z,A,S,y)

Uncertainties with the Metric

Moretto Nucl. Phys. A247 (1975) 211

$$\Gamma(y) dy = \frac{1}{2\pi\rho_{CN}(E^*)} \frac{\sqrt{2\pi T m_y}}{h} \int \rho[E^* - B(y) - \varepsilon] d\varepsilon \, dy$$

Moretto + Wozniak Prog. In Part. And Nucl. Phys. 21 (1988)

$$\Gamma(Z) = \frac{1}{2\pi\rho_{CN}(E^*)} \int \rho[E^* - B_Z - \varepsilon] d\varepsilon, Z = 3, 4, \dots, Z_{CN}/2$$

but why not

$$\Gamma(A) = \frac{1}{2\pi\rho_{CN}(E^*)} \int \rho[E^* - B_A - \varepsilon] d\varepsilon, A = 6, 7, \dots, A_{CN}/2$$

or

$$\Gamma(Z,A) = \frac{1}{2\pi\rho_{CN}(E^*)} \int \rho[E^* - B_{Z,A} - \varepsilon] d\varepsilon, A = 6,7,...,A_{CN}/2, Z = 3,4,..Z_{CN}/2$$

Now 3 dimenional. The latter is used in GEMINI and was also used in EDCATH [Mittig PRC **35** (1987)190]

Why does metric matter – effects the total fission width Sum over all asymmetries associated with the fission peak.

parabolic expansion
$$B(y) = B_f + \frac{1}{2}k y^2$$
, $y = \frac{A_1 - A_2}{A_1 + A_2}$
 $\Gamma_y^f = \int_{y\min}^{y\max} \Gamma(y) dy \approx \frac{1}{2\pi\rho_{CN}} \frac{\sqrt{2\pi Tm_y}}{h} \int_{-\infty}^{\infty} \int \rho \left(E^* - B_f - \frac{1}{2}ky^2 - \varepsilon\right) d\varepsilon dy$
use $\rho \left(E^* - \frac{1}{2}ky^2\right) \approx \rho \left(E^*\right) \exp\left(\frac{ky^2}{T}\right), \frac{1}{T} = \frac{d\rho}{dE^*}$
 $\Gamma_y^f \approx \frac{1}{2\pi\rho_{CN}} \frac{T}{\omega_b^y} \int \rho \left(E^* - B_f - \varepsilon\right) d\varepsilon = \frac{T}{\omega_b^y} \Gamma_{BW}, \quad \omega = \sqrt{\frac{k}{m_y}}$
 $\Gamma_Z^f = \sum_{Z\min}^{Z\max} \Gamma(Z) \approx \frac{T}{\omega_b^y} \frac{Z_{CN}}{2} \frac{h}{\sqrt{2\pi Tm_y}} \Gamma_{BW}$
 $\Gamma_A^f = \sum_{Z\min}^{Z\max} \Gamma(A) \approx \frac{T}{\omega_b^y} \frac{A_{CN}}{2} \frac{h}{\sqrt{2\pi Tm_y}} \Gamma_{BW}$
 $\Gamma_Z^{f} = \sum_{Z\min}^{\Sigma} \Gamma(Z, A) = ...$
 $A = 200, m_y = 636 \text{ MeV } zs^2, \quad \omega_b^y = .2 \text{ MeV}, \quad T = 1 \text{ MeV}$
 $\Gamma_y^f = 5 \Gamma_{BW}^f, \quad \Gamma_Z^f = 13 \Gamma_{BW}^f, \quad \Gamma_A^f = 33 \Gamma_{BW}^f, \quad \Gamma_Z^f = 65 \Gamma_{BW}^f$

Moretto's Solution Level densities dependent on the metric

$$\Gamma_{Z}^{f} == \Gamma_{A}^{f} == \Gamma_{y}^{f} == \Gamma_{BW}^{f}$$

$$\Gamma_{BW} = \frac{1}{2\pi\rho_{CN}} \int \rho^{BW} (E^{*} - B_{f} - \varepsilon) d\varepsilon$$

$$\Gamma(Z) = \frac{1}{2\pi\rho_{CN}} \int \rho^{Z} (E^{*} - B_{Z} - \varepsilon) d\varepsilon$$

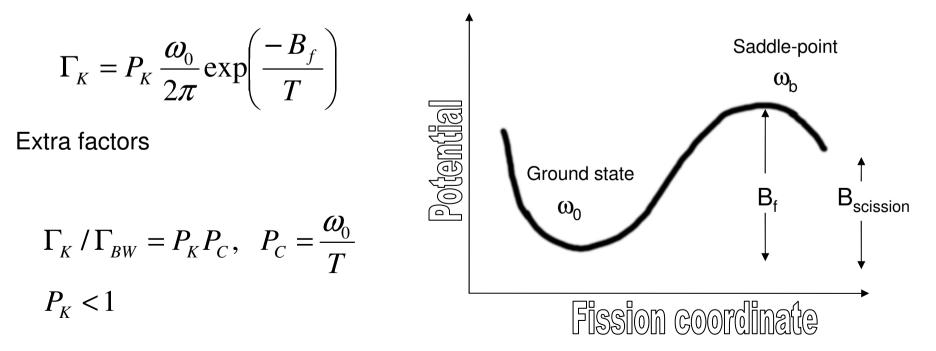
$$\rho^{Z} = \frac{\rho^{BW}}{\frac{\omega_{b}}{T} \frac{Z_{CN}}{2}} \sqrt{\frac{h}{2\pi T m_{y}}}$$

Which of ρ^z , ρ^A , ρ^y , ρ^{ZA} , or ρ^{BW} are Fermi-gas level densities What do you do for light nuclei where there is no fission peak? The transition-state formalism is an ansatz borrowed from chemistry where it is used to describe chemical reaction rates...

as
$$\rho(E^*-x) \approx \rho(E^*) \exp\left(\frac{x}{T}\right)$$

 $\Gamma_{BW} \approx \frac{1}{2\pi\rho(E^*)} \int \rho(E^*) \exp\left(\frac{B_f - \varepsilon}{T}\right) d\varepsilon \approx \frac{T}{2\pi} \exp\left(\frac{-B_f}{T}\right)$

In a one dimensional model, Kramers solved the problem for barrier crossing due to a random walk. Physica **7**, 284 (1940)

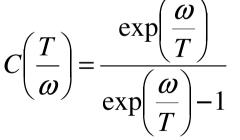


Collective enhancement factor ($P_C > 1$)[Strutinsky Phys. Lett. 47B, 121 (1960)] vibrations in ground state well

$$\rho *_{CN} (E*) \approx \iint \rho \left(E* -\frac{1}{2} kx^2 - \frac{p_x^2}{2m_x} \right) \frac{dx \, dp_x}{h}$$
$$= \frac{T}{\omega_0} \rho(E*) = C \left(\frac{T}{\omega_0} \right) \rho(E*) \quad \omega_0 = \sqrt{\frac{k}{m_x}}$$

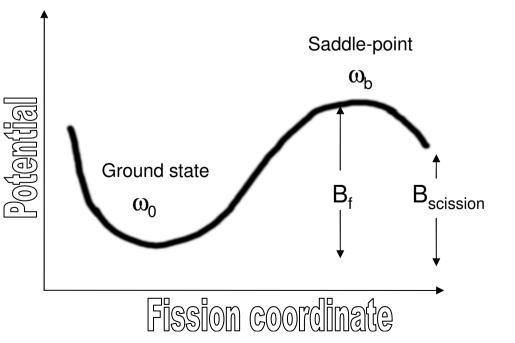
Classical result C=T/ ω_0 , T > ω_0

Quantum



If T< ω , C=1, mode is turned off

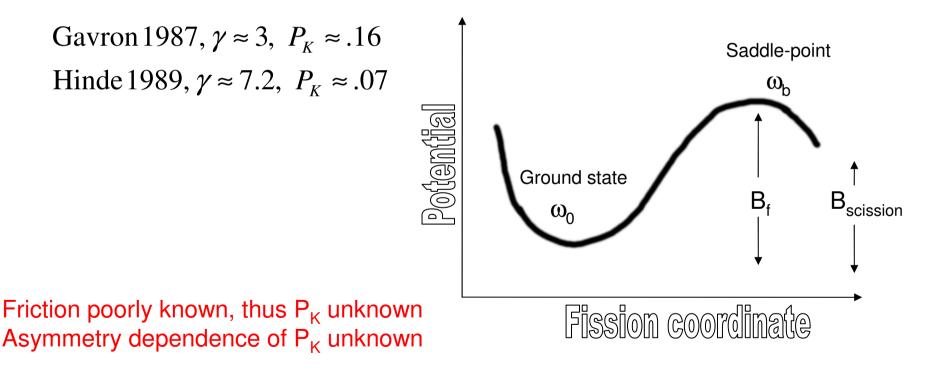
$$P_{C} = \frac{1}{C\left(\frac{T}{\omega}\right)} \le 1$$



Kramers' factor

(Large friction result)

$$P_{K} = \sqrt{\frac{\gamma^{2}}{4} + \omega_{b}^{2} - \frac{\gamma}{2}}, \gamma = \text{friction}, P_{K} < 1$$



No P_K or P_C in GEMINI $P_K < 1$, $P_C < 1$ (1-DIM)

Two dimension Kramers model (Jing-Shang+Weidenmuller)

$$\Gamma_{K}^{2d} = P_{K}^{2d} \frac{1}{2\pi\rho_{CN}^{**}(E^{*})} \int \rho^{*} (E^{*} - B_{f} - \varepsilon) d\varepsilon$$
$$\rho_{CN}^{**}(E^{*}) = \rho_{CN} C \left(\frac{T}{\omega_{0}^{x}}\right) C \left(\frac{T}{\omega_{0}^{y}}\right)$$
$$\rho^{*}(E^{*}) = \rho(E^{*}) C \left(\frac{T}{\omega_{b}^{y}}\right)$$

 P_{K}^{2d} is a complicated function of the friction tensor, inertia tensor, Hessian of the potential energy surface at the barrier,

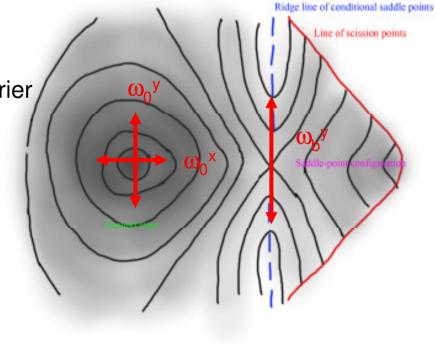
A = 200

 ω_0^x (quadrupole vib) = 1.4 MeV ω_0^{γ} (octapole vib) = 3.7 MeV

(Turned off)

$$\omega_b^y$$
 (fission asy) = 0.2 MeV
at T = 1

$$P_{C} = \frac{C\left(\frac{T}{\omega_{b}^{y}}\right)}{C\left(\frac{T}{\omega_{0}^{x}}\right)C\left(\frac{T}{\omega_{0}^{y}}\right)} = 4.07 \ge 1, P_{K} < 1 (2 - \dim)$$



Multi dimensional model

$$P_{C} = \frac{\prod_{i=1}^{N-1} C_{i}^{\text{saddepoint}}}{\prod_{i=1}^{N} C_{i}^{gs}}$$

ground state : A = 200, $\omega_{hexadecapole}$ = 6.76 MeV, other higher order modes have larger frequencies. The ground state collective vibrations are turned off, except for the quadrupole mode, $C_{i>1}^{gs} = 1$

Saddle - point has many more (turned on) collective modes,

 P_{C} increases if we go to higher dimensions

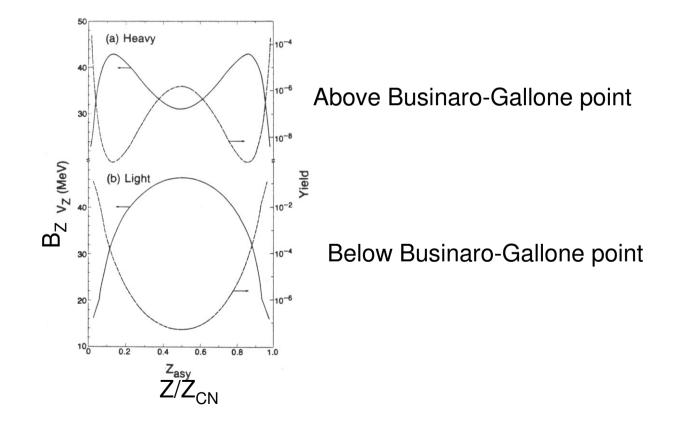
There are angular momentum baring modes at the saddle point (wriggling, bending, tilting, twisting) which should further enhance level density and P_c

 $P_{K} < 1$, $P_{C} > 1$ – maybe they cancel?

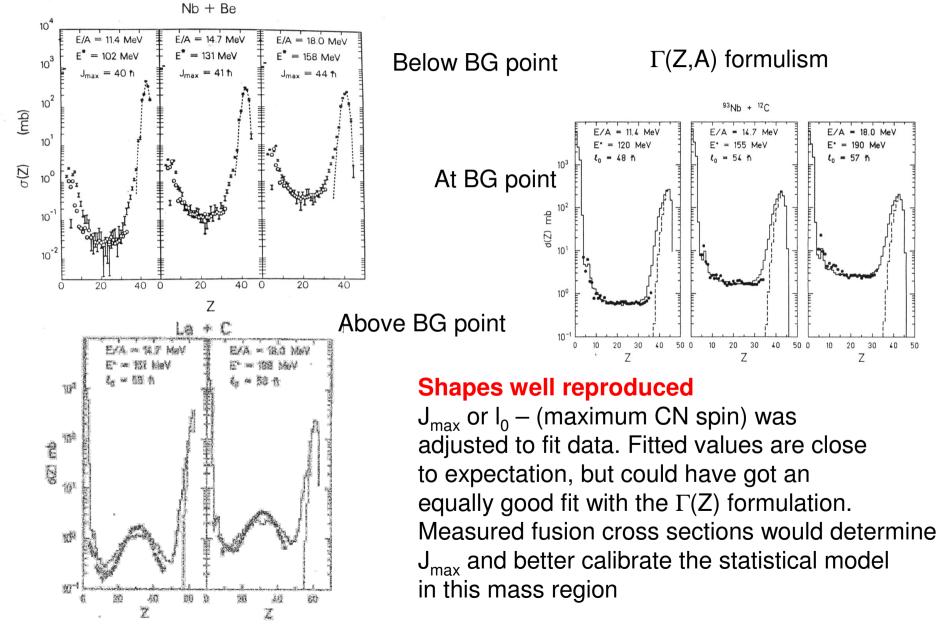
- Results for symmetric and asymmetric fission dependent on the dimensionality of the calculation.
- How many dimensions to work in ? A free parameter of the model.
- The dimensionality will change with mass number
- One approach will not work for all masses
- The extent that the Bohr-Wheeler formulism works is probability due to cancellation of the $\rm P_K$ and $\rm P_C$ factors

Charge or mass distribution is a refection of the potential energy surface

$$\Gamma(Z) \propto \rho(E^* - B_Z) \approx \rho(E^*) \exp\left(\frac{-B_Z}{T}\right), T = \text{temperature}$$



Comparison of GEMINI to heavy-ion fusion data E* known well, angular momentum distribution poorly known



Increasing angular momentum has the same effect as increasing the mass

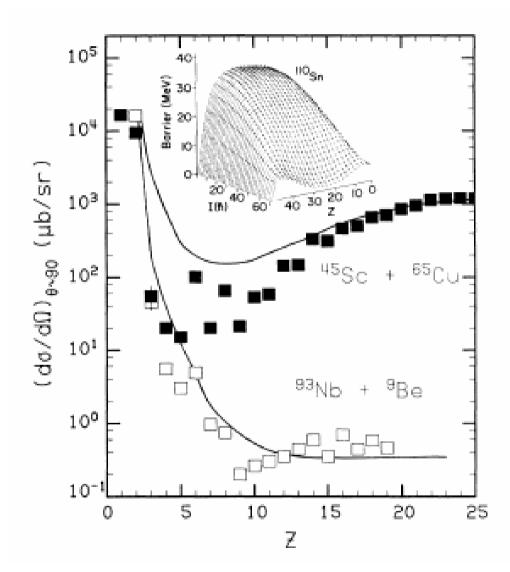
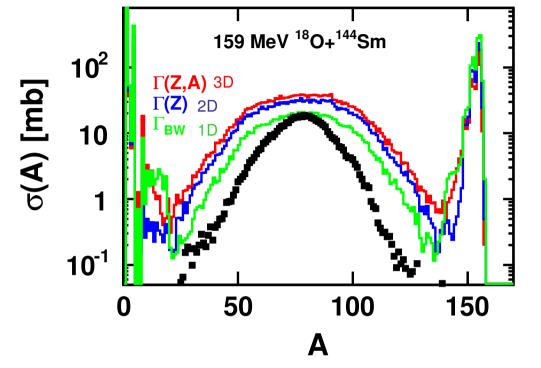


TABLE L	Ouantities	characterizing	the reactions of	interest.
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System	E _{lab} (MeV)	CN	E* (MeV)	I_{ent}^{a} (\hbar)	/ ^b	x°	уª
⁹³ Nb+ ⁹ Be	782	¹⁰² Rh	78	34	43	0.40	0.05
⁴⁵ Sc+ ⁶⁵ Cu	200	¹¹⁰ Sn	94	70	80	0.45	0.17

Sobotka et al PRC 36, 2713 (1987)



Standard GEMINI [I (\angle ,A)] over predicts the fission yield – The Γ_{BW} formulism does much better – but still too big Need recalibration for this mass region

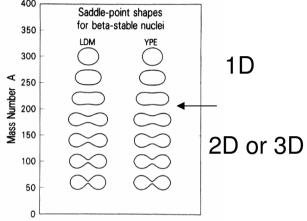
For fissile compound nuclei GEMINI overpredicts the width of the fission mass distributions

- a) temperature at saddle point is colder than GEMINI predicts?
- c) problem with the asymmetry dependence of barriers?
- b) saddle-scission transition modifies distribution?

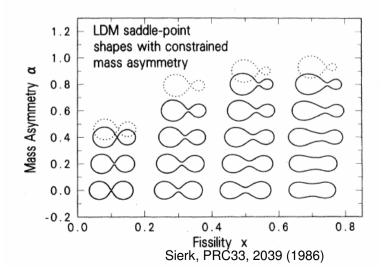
$$\Gamma_Z \propto \exp\left(-\frac{B_Z}{T}\right)$$

GEMINI assumes the saddle and scission point are degenerate.
a) excitation at scission is divided between the two fragments. No dissipation of energy between the saddle and scission
b) mass asymmetry at saddle and scission are identical. No fluctuations in asymmetry between saddle and scission

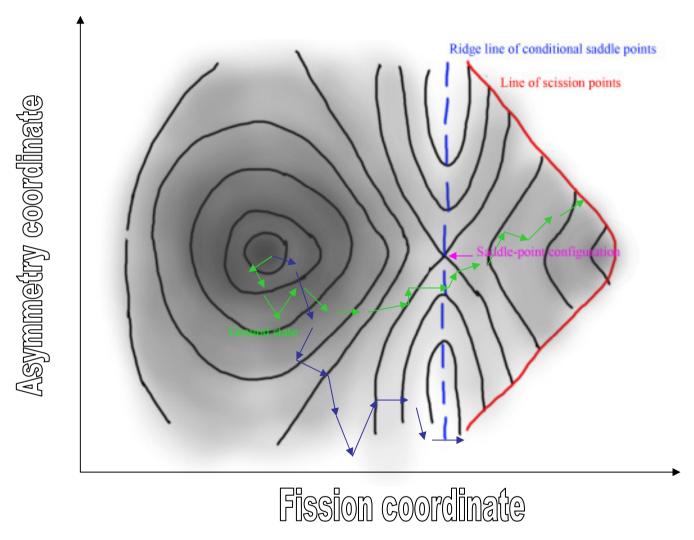
This is reasonable when the saddle-point has a well defined neck – short saddle-to scission distance Bad Assumption for symmetric division of heavy systems. For very heavy systems, there is not neck and the asymmetry parameter is not defined at all.



Thomas, Davies, + Sierk, Phys. Rev. C31, 915 (1985)



Potential energy surface



For large saddle-to-scission distance asymmetry at saddle may not be preserved at scission

Another formulism – Scission-point logic instead of saddle-point

Scission-point model of nuclear fission based on deformed-shell effects Wilkins, Steinberg and Chasman, PRC 14, 1832 (1976)

Fission mass distribution determined from a thermal model at scission Scission-point energy determined from touching spheroids with shell corrections

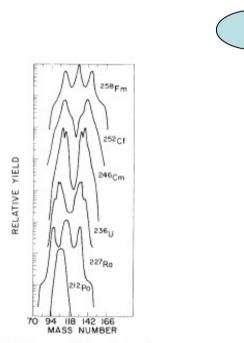
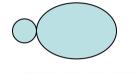


FIG. 8. Calculated mass-yield distributions for various fissioning systems using a single set of parameters ($T_{\rm coll}$ = 1.0 MeV, $\tau_{\rm int}$ = 0.75 MeV and d = 1.4 fm) for all systems.



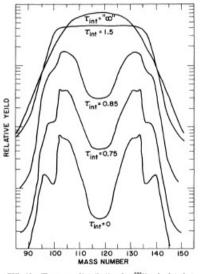
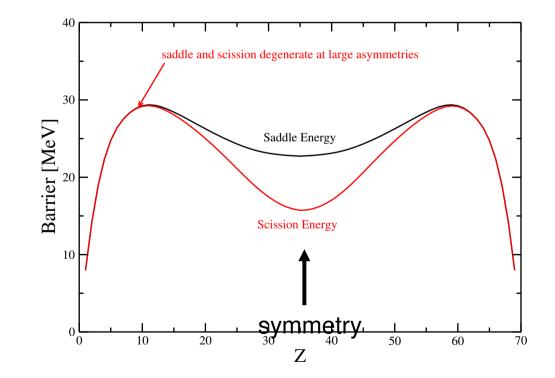
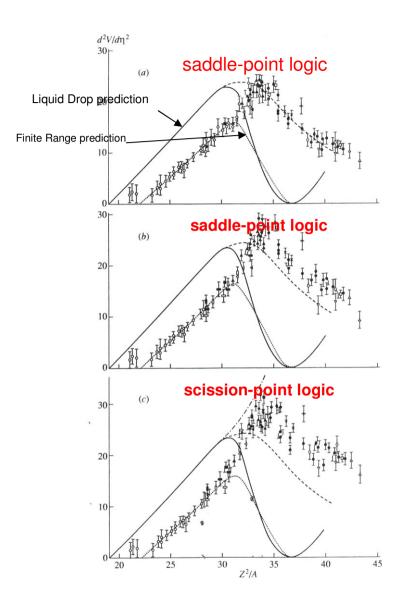


FIG. 11. The mass distribution for ²³⁶U calculated at several different temperatures τ_{int} . The calculation at $\tau_{int} = -\infty$ has the shell and pairing corrections set to zero.

Light systems saddle-point and scission point model are degererate

Stiffness $(d^2V/dZ^2)_{sym}$ at scission point should be larger than that at saddle for a heavy system so a scission-point logic would predict narrower barrier distributions than a saddle-point logic





Systematic of fission mass distributions (no double-humped distributions)

Rusanov, Itkis, Okolovich, Phys. Atomic. Nucl. 60,683 (1997)

asymmetry stiffness = $\frac{d^2 V}{d\eta^2} = A_{CN} \frac{T}{16\sigma_M}$

 σ_{M} = standard deviation of fission mass distribution

The stiffness in the stiffness at the saddle or scission points, depending on which logic one used.

T (temperature) determined after accounting for presaddle and or saddle-to-scission neutrons emitted.

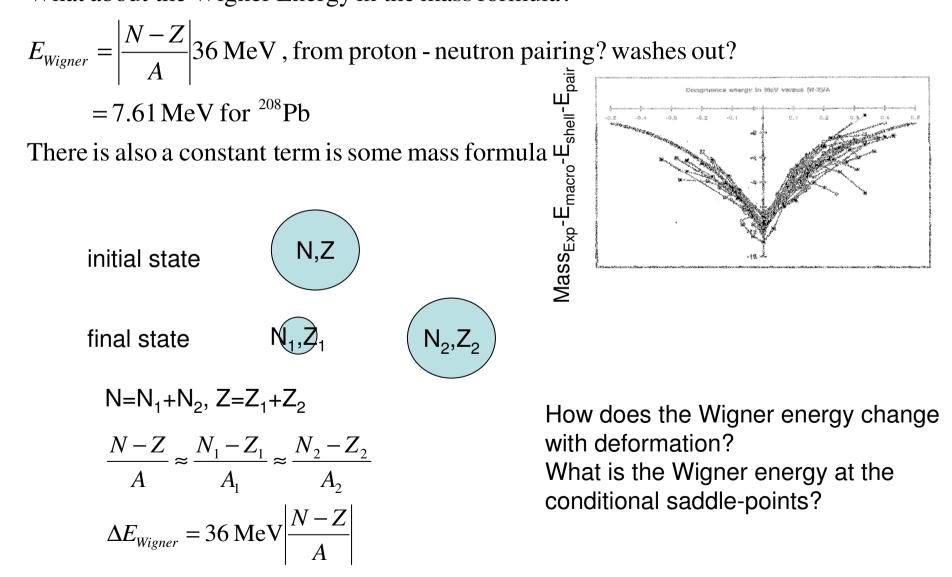
From measured $\sigma_{\mbox{\scriptsize M},}$ (corrected for angular momentum), deduce stiffness.

As a practical matter, could use these stiffnesses and statistical model values of T to predict the mass distributions – interpolation from the systematics.

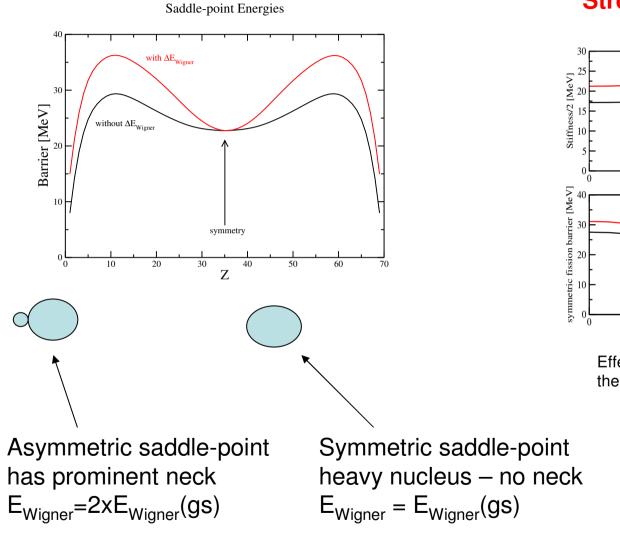
Is the asymmetry dependence of conditional saddle-point energies correct in GEMINI?

Saddle-point energies are often calculated as $\Delta E_{Coulomb} + \Delta E_{Surface}$ For example the Sierk's calculations used by GEMINI

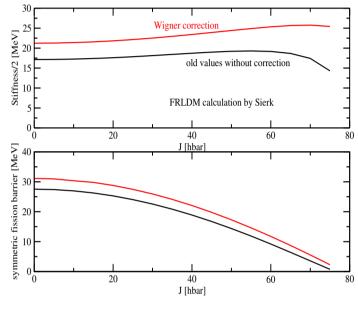
What about the Wigner Energy in the mass formula?



schematic



Wigner correction make asymmetry dependence Stronger.



Effect not large enough to fully explain the ¹⁶²Yb results

Inclusion of Wigner Energy will give narrower mass distributions?

Fission dynamics

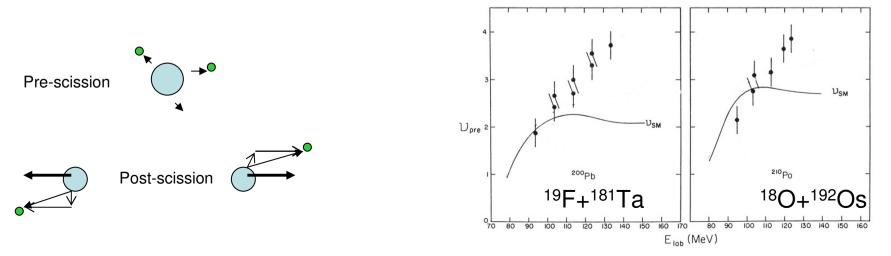
Pre and post-scission multiplicities of light particles are sensitive probes to the fission dynamics.

Motion along the fission coordinate is slow and highly dissipative (over damped) for symmetric fission.

Large friction – large fluctuations (fluctuation dissipation theorem)

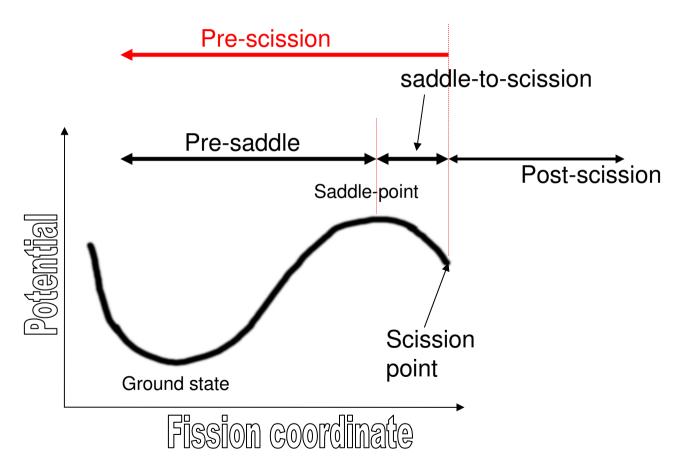
Post-scission multiplicities->The excitation energy at the scission point is 0.2 to 0.4 MeV/A independent of the initial compound-nucleus excitation energy. 40-80 MeV for A=200 [Hilscher and Rossner Ann. Phys. Fr. **17** (1992) 471]

Pre-scission neutron multiplicities cannot be explained with the standard statistical model (GEMINI) without dynamics



To explain experimental pre-scission multiplicities need

- a) More pre-saddle emission fission transients and/or
- b) saddle-to-scission emissions



Fission transients

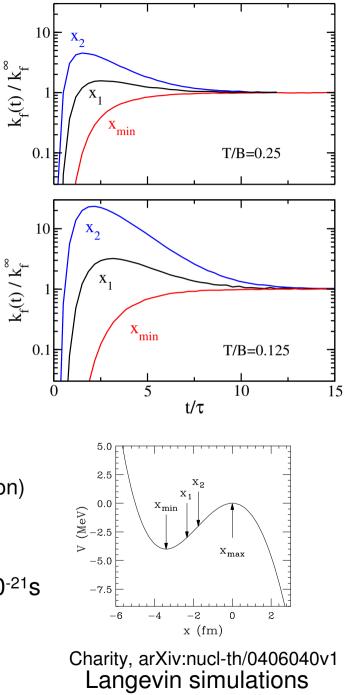
Compound-nucleus decay widths are appropriate for a system equilibrated in all of its degrees of freedom. The Kramers' fission rate assumes the collective or shape degrees of freedom are in equilibrium.

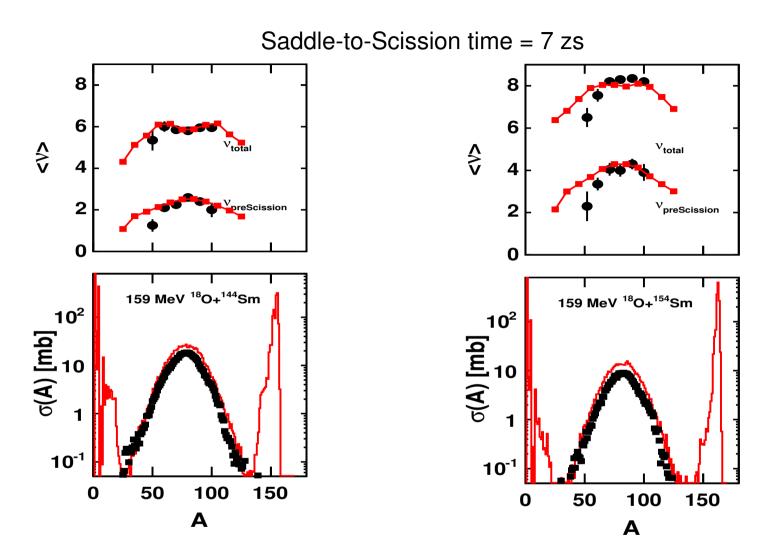
It takes a finite time (transient time) for the equilibrium to occur. The transient fission rate can be larger or smaller than the equilibrium depending on the initial conditions.

Most studies assume an initial suppression of fission (fission delay) – during which light particle emission can occur and cool the system and reduce fission probability.

GEMINI incorporates a simplistic fission decay (step function) Γ_{Z} = 0 for time < $t_{transient}$

C. Schmitt et al., PRL **99** 042701 (2007) transient time for initially spherical systems= 3.3×10^{-21} s K.X. Jing PLB **518**, 221 (2001) 10×10^{-21} s Doesn't have much affect for the data I showed.





Modification to GEMINI that uses a scission-point model. Asymmetry-dependence of scission potential from touching spheres. Evaporation of neutrons from saddle-to-scission.

Conclusions

- GEMINI has the correct treatment of angular momentum
- GEMINI seems to work reasonable well for light compound nuclei, but I am not sure why.
- GEMINI doesn't work for heavy systems-problems with the fission yield and width of mass distribution

a) few dimensions

b) new barriers will help (Wigner Correction?)

c) Could interpolate from systematic of fission mass distributions after including fission delays and saddle-to-scission time.

d) A simplistic scission-point model for mass distributions gives good results (could include shell effects to get double humped distributions)

- Lower Coulomb barriers for alpha + Li+Be. emission for heavy systems
- Large temperature dependence of level-density parameter for heavy systems