Fission properties in a static self-consistent mean-field approach

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Introduction

Motivations

- Need for improved theory of fission in neutron-induced cross-section calculations at low energy for actinides (GNEP/AFC programs)
- Better understanding of the mechanisms responsible for the fission-fragment properties (angular momentum, deformation, excitation)
- Assessment of the capabilities of current microscopic approaches, here the Skyrme–Hartree–Fock-BCS model

Outline

- *n*-induced fission cross sections
- Fission properties from the potential-energy surface
- Fission-fragment angular momentum

Cross sections

Fission cross section

- Bohr independence hypothesis: $\sigma_{nf}(E) = \sum_{J,\pi} \sigma_{\mathrm{CN}}^{J^\pi} P_f^{J^\pi}$

  (if no width fluctuations) with $\sigma_{\mathrm{CN}}^{J^\pi} = \frac{\pi}{k_n^2} \frac{2J+1}{2(2I_T+1)} T_n^{J^\pi}$
- Fission probability for double-hump fission barriers
  - Hauser-Feshbach expression (GNASH, TALYS):

$$P_f^{J^\pi} = \frac{T_f}{T_f + T'} \ , \ T_f = \frac{T_A T_B}{T_A + T_B} \ , \ T' = T_n + T_\gamma + \ldots$$

  - Lynn-Back expression (EMPIRE):

$$P_f^{J^\pi} = \frac{T_{\mathrm{dir}}}{T_{\mathrm{dir}} + T'} \left\{ 1 + \frac{T'}{T_{\mathrm{dir}}} \left[1 + R^2 + 2R \coth\left(\frac{T_A + T_B}{2} \right) \right]^{-1/2} \right\}$$

  with $R = (T_{\mathrm{dir}} + T')(T_A + T_B)/(T_{\mathrm{abs}} T_B)$

Cross sections

Fission transmission coefficient

- Needed for all reactions (not only fission cross sections)
- Current approaches in reaction codes (GNASH, TALYS, EMPIRE,...):
  - one-dimensional multi-humped parabolic barrier
  - Hill–Wheeler penetrability of each hump (constant mass parameter)
- Extensions: include more fission properties
  - realistic fission-barrier profile
  - multidimension effects: coupling of several degrees of freedom (elongation, mass asymmetry, ...)
  - multimodal fission (several paths to scission)

$\Rightarrow$ What can we learn about these fission properties with a static, self-consistent mean-field model? (here, HFBCS)

Fission properties

Fission-process properties

- Fission barrier heights
- Fission modes (transition ^{256}Fm $\rightarrow$ ^{258}Fm in spontaneous fission)
- Fission half-lives

...

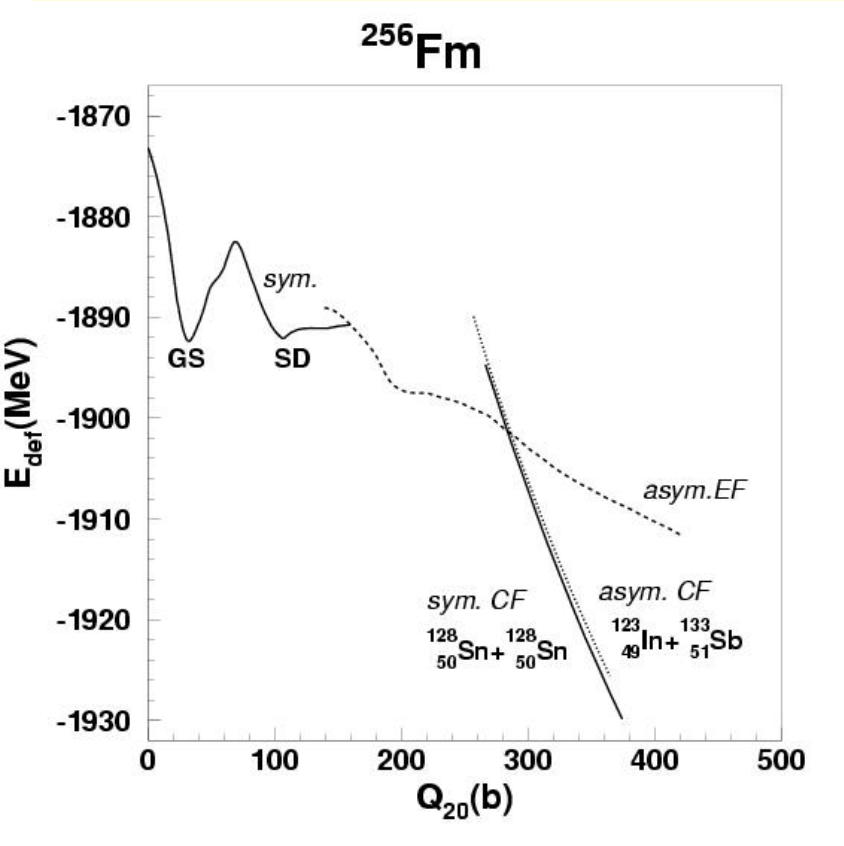
Fission-fragment properties

- Mass, kinetic energy, angular momentum distributions...
- Theoretical issues:
  - Definition of scission
  - Scission configuration probability
  - Angular momentum generation mechanism (orientation pumping, ^{252}Cf $\xrightarrow{\text{SF}}$ ^{106}Mo+^{146}Ba)

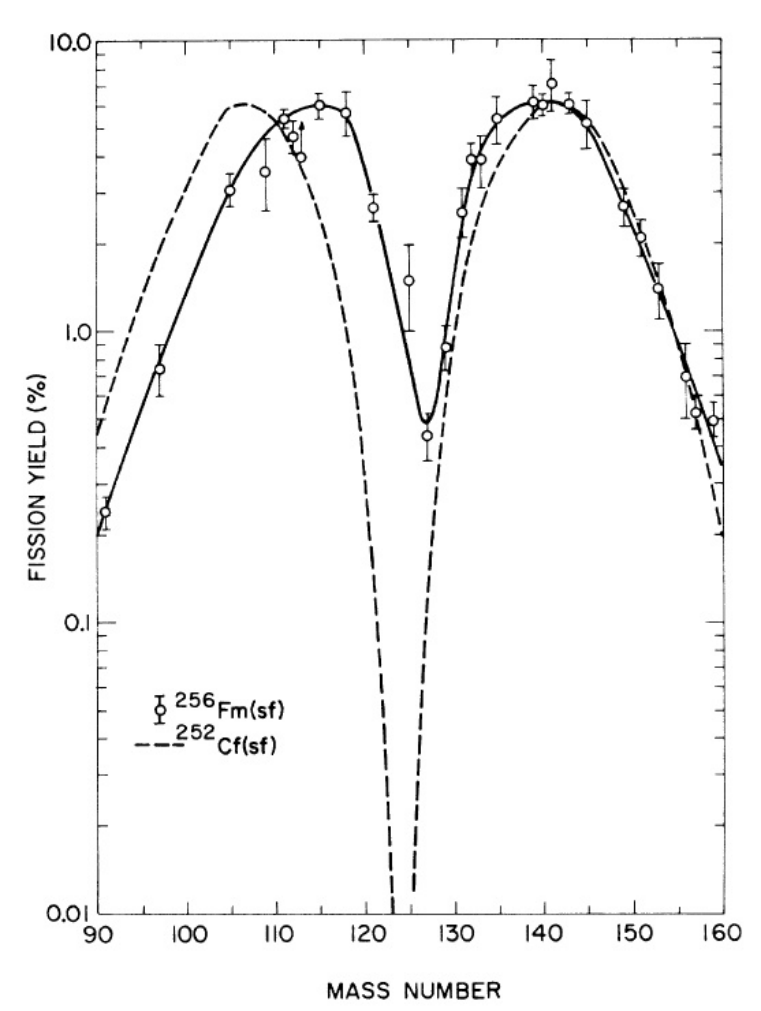
Fission modes of ^{256}Fm and ^{258}Fm

^{256}Fm

L.B., PRC 74 (2006)

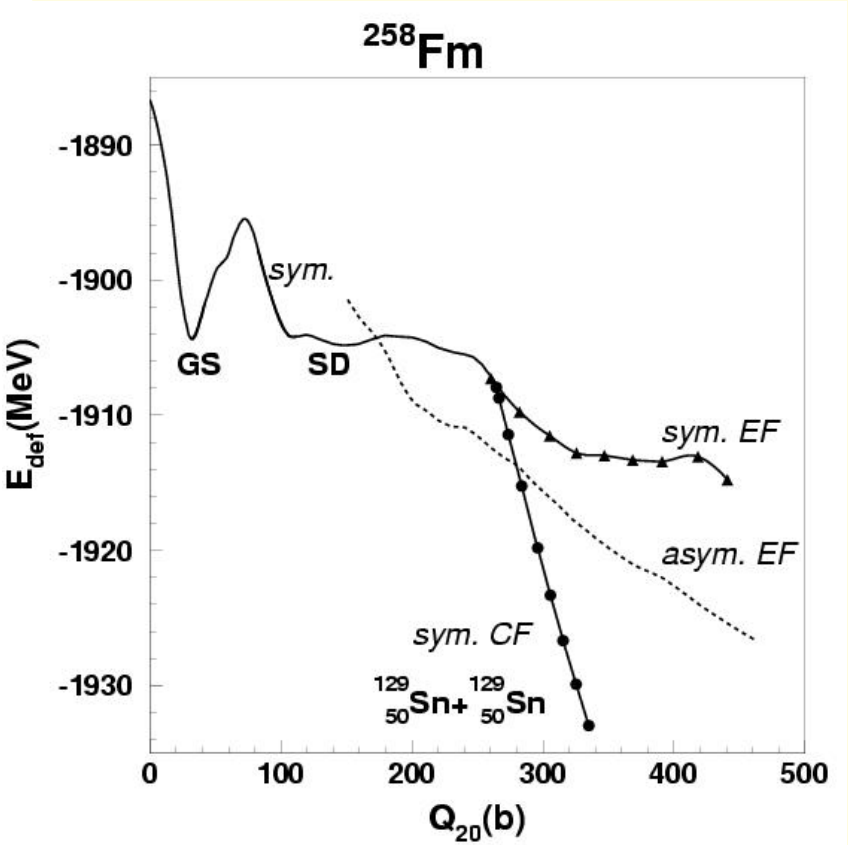


Flynn *et al.*, PRC 5 (1972)

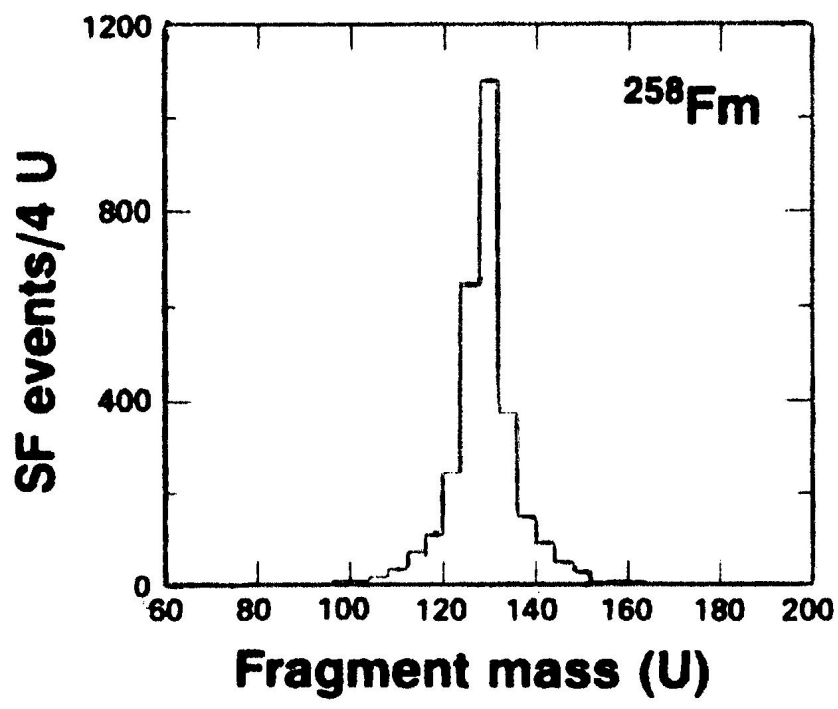


Fission modes of ^{256}Fm and ^{258}Fm

^{258}Fm

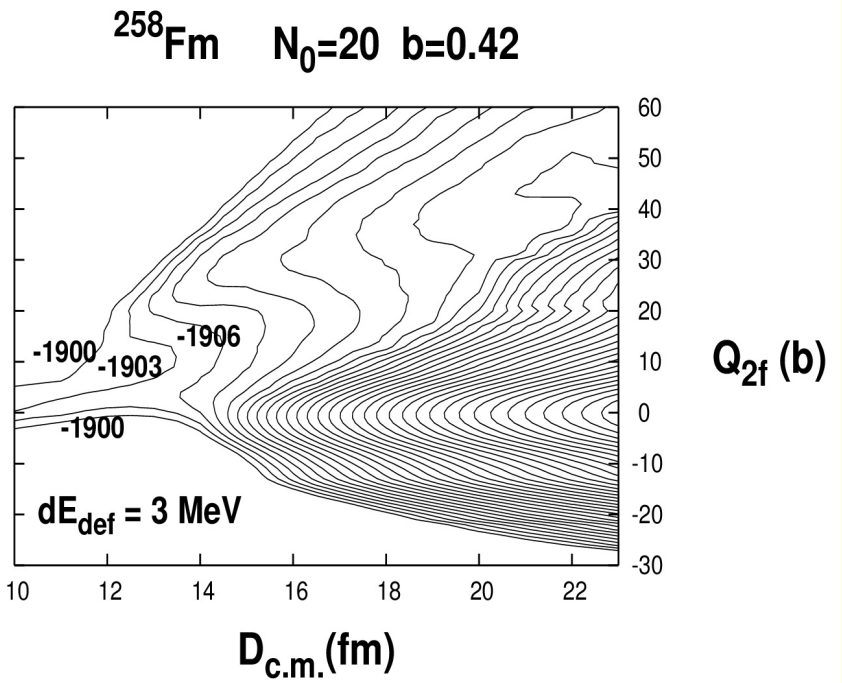


Hulet *et al.*, PRL 56 (1986)

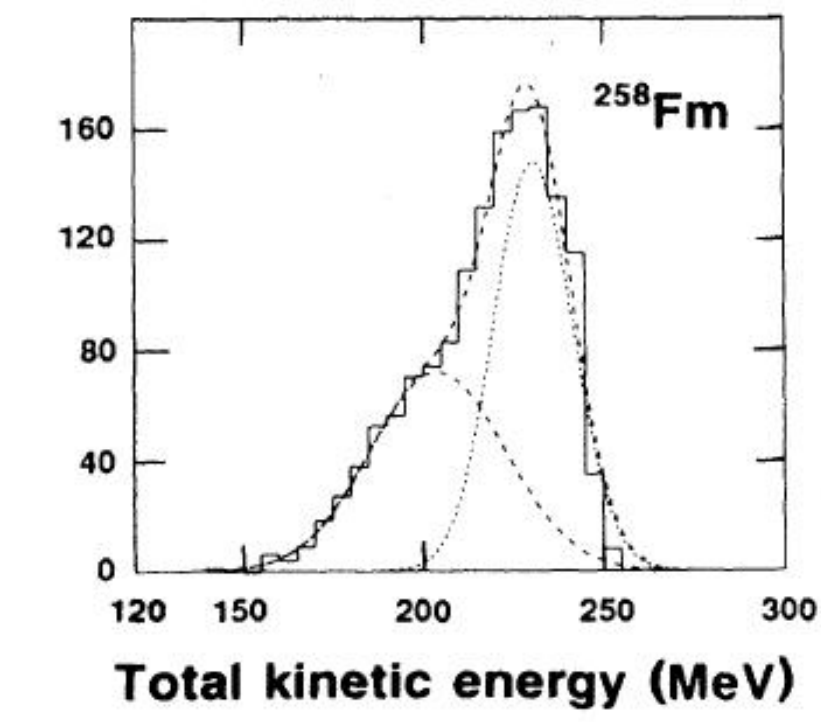


Fission modes of ^{256}Fm and ^{258}Fm

Bimodal fission of ^{258}Fm



Hulet *et al.*, PRC 40 (1989)



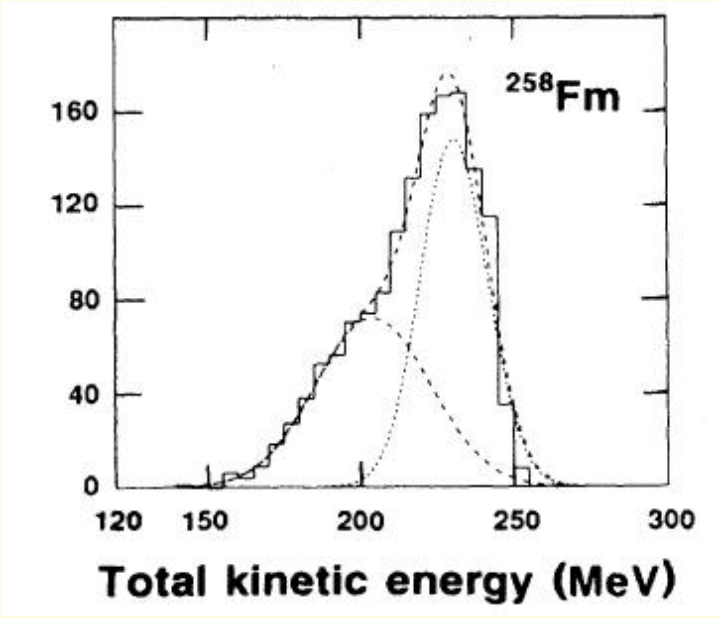
Valleys stable against mass asymmetry (depth not calculated here)

Fission modes of ^{256}Fm and ^{258}Fm

Bimodal fission of ^{258}Fm

- calculated values of TKE for each path (in MeV):

valley	TKE
sym. CF	244
asym. EF	215
sym. EF	184



- compatible with experiment
- interpretation of fission modes:
  - high-TKE mode: sym. CF
  - low-TKE mode: sym. EF + asym. EF

Fission modes of ^{256}Fm and ^{258}Fm

Bimodal fission of ^{258}Fm

- calculated values of TKE for each path (in MeV):

valley	TKE
sym. CF	244
asym. EF	215
sym. EF	184

- experimental modes: mean and width (in MeV)

mode	$\overline{\mathrm{TKE}}$	σ_{TKE}
high-TKE	230	16
low-TKE	205	27

- compatible with experiment
- interpretation of fission modes:
  - high-TKE mode: sym. CF
  - low-TKE mode: sym. EF + asym. EF

Fission-fragment spin

Experimental facts

- Sizeable angular momentum carried out by fission fragments in low-energy fission, even spontaneous fission of even-even nuclei in their GS ($\approx 8\,\hbar$ for ^{252}Cf)
- Observation of γ-deexcitation of fragments in competition with neutron emission, which carries out little spin (EUROBALL, GAMMASPHERE 4π Ge arrays)
- Very difficult to infer primary-fragment spins ; uncertainties of the order of 2 $\hbar$

Theoretical challenge

- Reasonable goal: reproduction of order of magnitude and trends (with fragment excitation energy, fragmentation, ...)
- Several possible sources of fragment spin;here, orientation pumping (Heisenberg principle)

FISSION-FRAGMENT SPIN

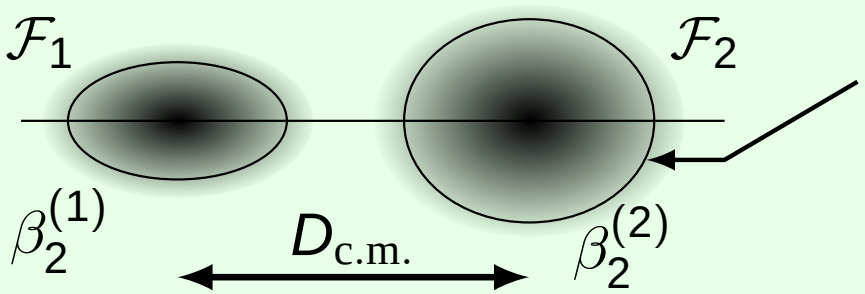
ORIENTATION PUMPING

- Primary fragments acquire angular momentum at scission
- The intrinsic state describing a scission configuration is a physical state
- Heisenberg principle: well-defined orientation in space (fission direction) $\Rightarrow$ distribution of angular momentum in the perpendicular plane $\Rightarrow$ finite angular momentum of fragments
- Testing this mechanism alone: discarding any other source of angular momentum
- Minimal scheme: spontaneous fission of an even-even nucleus in its GS

I. N. Mikhailov and P. Quentin, PLB 462,7 (1999)

FISSION-FRAGMENT SPIN

DESCRIPTION OF SCISSION CONFIGURATIONS



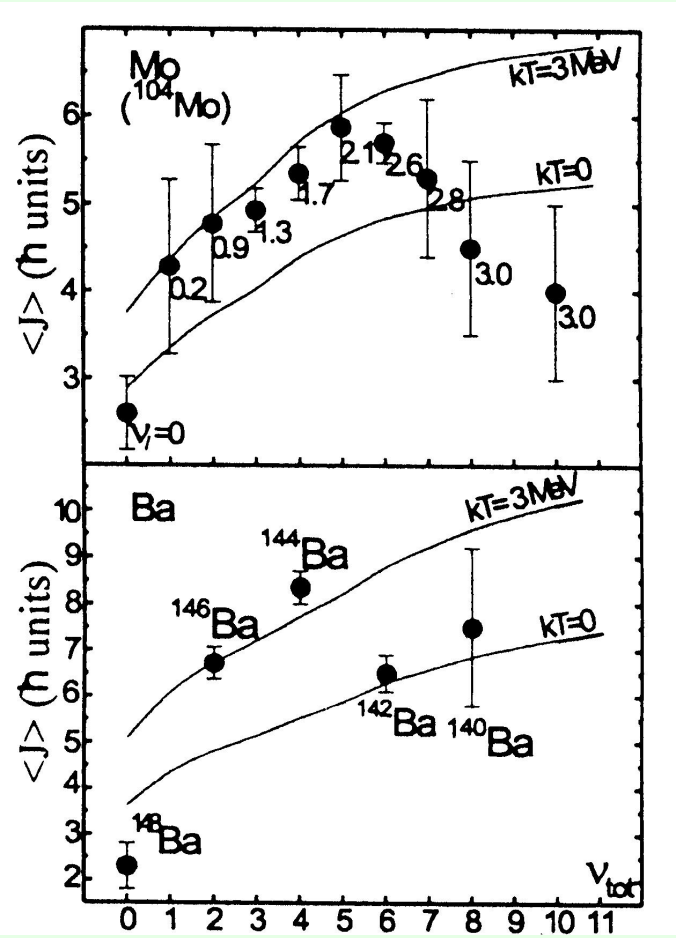
equivalent spheroid (same deformation and size)

- Scission-configuration energy: $E_{\text{SC}} = E_C + E_N + \sum_i E_{\text{SC}}^{(i)}$
- Mutual polarization neglected
- Fragment deformation energies: $E_{\text{DEF}}^{(i)} = E_{\text{SC}}^{(i)} - E_{\text{GS}}^{(i)}$
  - HF(SkM*)+BCS(G) approach
  - axial and left-right reflection symmetries assumed
- Coulomb and nuclear interaction energies between equivalent spheroids: E_C: exact, E_N: YPE potential

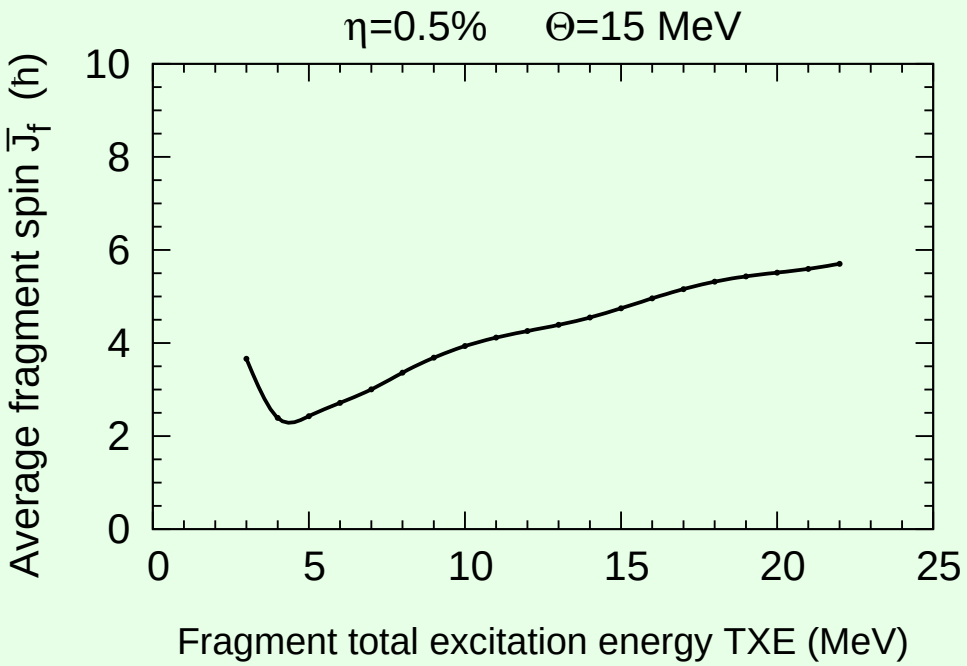
FISSION-FRAGMENT SPIN

COMPARISON WITH EXPERIMENT

Application to $^{252}\mathrm{Cf} \longrightarrow {}^{106}\mathrm{Mo} + {}^{146}\mathrm{Ba}$



G. M. Ter Akopian et al., *Proc. of the 3rd Int. Conf. on Fission [...]* (1999) p. 98.



$$\overline{\nu}_{\mathrm{tot}} \approx \frac{\mathrm{TXE}-5.5}{5.5+1.5}$$

order of magnitude and globally increasing trend reproduced (L. B., P. Quentin and I.N. Mikhailov, submitted to PRC)

CONCLUSION

- Very encouraging results on fission properties from the static self-consistent mean-field approach HF(SkM*)+BCS(G)
- Orientation pumping important for deformed fragments at low energy
- Need to treat dynamics to predict scission-configuration distributions ($\Rightarrow$ mass, TKE and spin distributions)
- Perspectives: more realistic calculations of fission barrier penetrability as input to cross section calculations (realistic barriers, multimodal fission, level densities at barrier top, ...)

Additional slides

Fission-fragment spin

Definition of scission

Moment of the fission process when nucleon dynamics in both fragments decouple and are externally influenced by the Coulomb interaction only

Quantitative formulation

- Dynamics $\Rightarrow$ forces between nucleons in different fragments: non-unique criterion
- Resulting forces between fragments: ratio of the nuclear and Coulomb forces $|\mathbf{F}_N|/|\mathbf{F}_C| = \eta \ll 1$
  $\mathbf{F}_N$ difficult to calculate
- Interaction energies between fragments: ratio of the nuclear and Coulomb interaction energies $|E_N/E_C| = \eta$

FISSION-FRAGMENT SPIN

ENERGY BALANCE

- Conservation of the total energy of the fissioning nucleus
- Spontaneous fission from the GS $\Rightarrow E_{\mathrm{TOT}} = E_{\mathrm{GS}}$
- Available energy at scission $E_{\mathrm{FREE}} \equiv E_{\mathrm{TOT}} - E_{\mathrm{SC}}$ shared between:
  - pre-scission kinetic energy $E_{\mathrm{K}}^{(\mathrm{sc})}$
  - intrinsic excitation energy $E_{\mathrm{T}}^{(\mathrm{sc})}$ (potential energy dissipated into intrinsic degrees of freedom) $\Rightarrow$ fragment temperature
  - unknown partitioning: $E_{\mathrm{K}}^{(\mathrm{sc})} = f\, E_{\mathrm{FREE}}$
- Energy released $Q = \mathrm{TKE} + \mathrm{TXE}$:
  - total kinetic energy $\mathrm{TKE} = E_C + E_N + E_{\mathrm{K}}^{(\mathrm{sc})}$
  - total excitation energy $\mathrm{TXE} = E_{\mathrm{DEF}} + E_{\mathrm{T}}^{(\mathrm{sc})}$
    ($E_{\mathrm{DEF}} = \sum_i E_{\mathrm{DEF}}^{(i)}$ total fragment deformation energy)

FISSION-FRAGMENT SPIN

FORMALISM OF IMPLEMENTATION

- Factorization of the fissioning-nucleus state into two HFBCS fragment states $|\Psi_i\rangle$:
$$|\Psi\rangle = |\text{relat. motion}\rangle \otimes |\Psi_1\rangle \otimes |\Psi_2\rangle$$
- Deformed fragments (ax. sym. assumed) $\Rightarrow |\Psi_i\rangle$ is not a good-J state: $|\Psi_i\rangle = \sum_{J \geqslant |K_i|} a_J^{(i)} |JK_i\rangle$
- Coupling and projection onto $J = 0$
- Rigid rotor approximation: $a_J^{(i)} \propto \exp\left(-\frac{J(J+1)}{\langle \mathbf{J}^2 \rangle_i}\right)$, with $\langle \mathbf{J}^2 \rangle_i = \langle \Psi_i | \mathbf{J}^2 | \Psi_i \rangle$
- Expectation value of $\mathbf{J}_i^2$ in $|\Psi\rangle$:
$$\langle \Psi | \mathbf{J}_i^2 | \Psi \rangle \approx \left(\frac{1}{\langle \mathbf{J}^2 \rangle_1} + \frac{1}{\langle \mathbf{J}^2 \rangle_2} \right)^{-1}$$
- Equal fragment spins J_F such that $J_\mathrm{F}(J_\mathrm{F}+1) = \langle \Psi | \mathbf{J}_i^2 | \Psi \rangle$

FISSION-FRAGMENT SPIN

FRAGMENT ANGULAR MOMENTUM AS A FUNCTION OF TXE

- Set of scission configurations:
  - scission criterion: $\left|\frac{E_N}{E_C}\right| = \eta \Rightarrow D_{\mathrm{c.m.}}$ function of $\beta_2^{(1)}$ and $\beta_2^{(2)}$)
  - accessible configurations: $E_{\mathrm{FREE}} \geqslant 0$ (below the GS)
  - fixed TXE

  $\Rightarrow$ restricted 1D space (1 curvilinear abscissa)
- Average over scission configurations for a given fragmentation:

$$\overline{J_{\mathrm{F}}} = \frac{1}{\mathcal{N}} \int_{\mathcal{C}_{\mathrm{TXE}}} ds\, J_{\mathrm{F}}\left(\beta_2^{(1)}(s), \beta_2^{(2)}(s)\right) w(s)$$

- Scission-configuration distribution in the collective space: quantal fluctuations around the minimum of E_{SC} roughly quadratic in $\beta_2^{(i)}$ $\Rightarrow w(s) \propto \exp(-E_{\mathrm{SC}}/\Theta)$
  characteristic width Θ estimated to be $\approx$ 1 MeV

Application to ^{252}Cf $\longrightarrow$ ^{106}Mo + ^{146}Ba

Average prompt-neutron multiplicity

- Fragment deexcitation by n and γ emission:

$$\mathrm{TXE} = \sum_{i=1}^{2} \left[\sum_{\nu=0}^{\nu_{\mathrm{tot}}} \left(S_n^{(i,\nu)} + \epsilon_n^{(i,\nu)} \right) + E_\gamma^{(i)} \right]$$

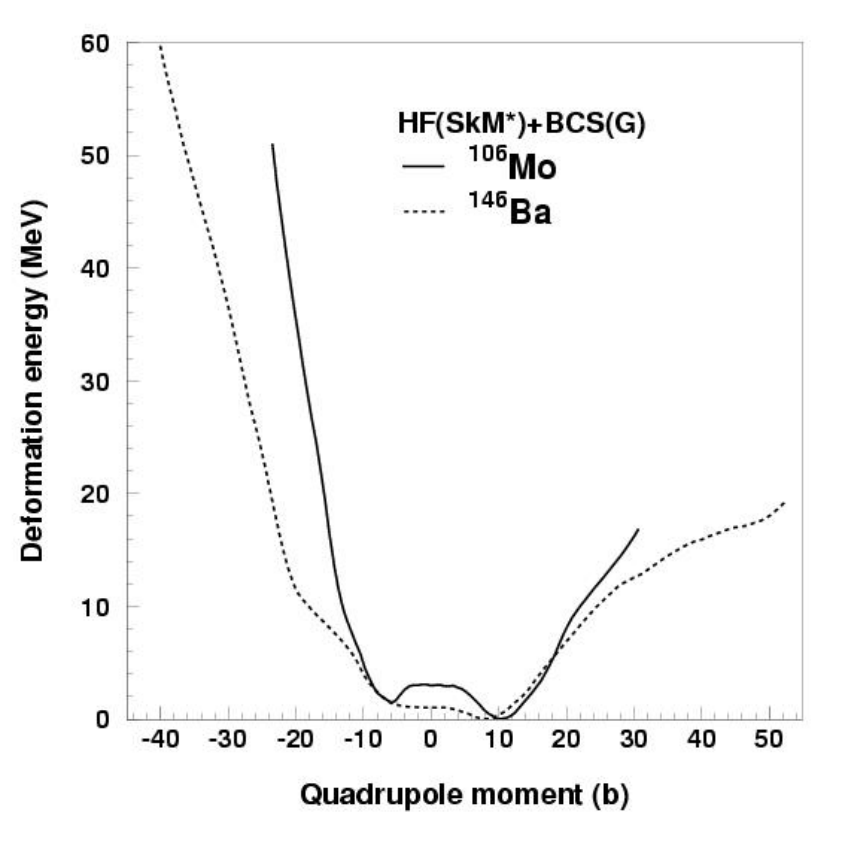
S_n : neutron separation energy ; ϵ_n : neutron kinetic energy

- Rough estimate of $\overline{\nu}_{\mathrm{tot}}$ as a function of TXE : no $n-\gamma$ competition assumed

$$\left.\begin{array}{r} \overline{S_n^{(i,\nu)}} \approx 5.5 \text{ MeV} \\ \overline{\epsilon_n^{(i,\nu)}} \approx 1.5 \text{ MeV} \\ \overline{E_\gamma^{(i)}} \approx \overline{S_n^{(i,\nu)}}/2 \end{array}\right\} \Rightarrow \overline{\nu}_{\mathrm{tot}} \approx \frac{\mathrm{TXE} - 5.5}{7.0}$$

Application to $^{252}Cf \longrightarrow {}^{106}Mo + {}^{146}Ba$

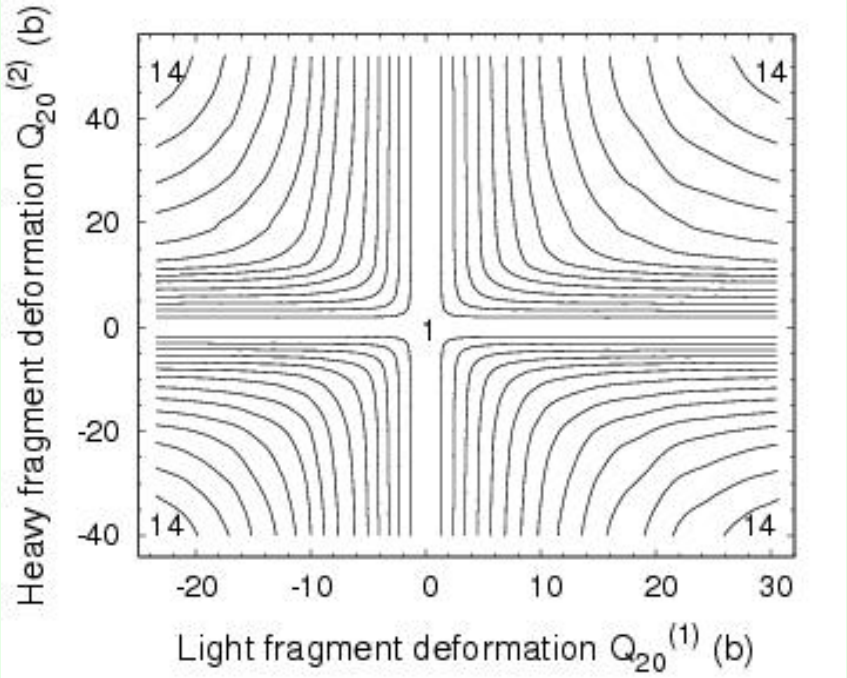
Fragment deformation energy



- ^{106}Mo : prolate GS + oblate minimum, rigid nucleus
- ^{146}Ba : prolate GS, soft nucleus

Application to ^{252}Cf $\longrightarrow$ ^{106}Mo + ^{146}Ba

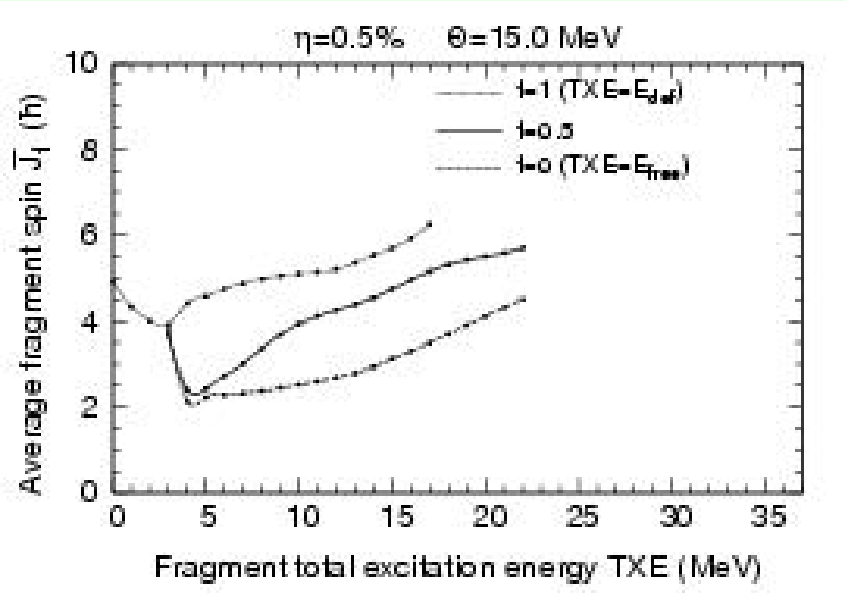
Fragment spin in the fragment-deformation plane



- $J_F = 0$ when one of the fragments is spherical
- Intrinsic expectation value $\langle \mathbf{J}^2 \rangle_i \approx$ quadratic function of deformation
- Contours of fragment spin $\approx$ hyperbolas

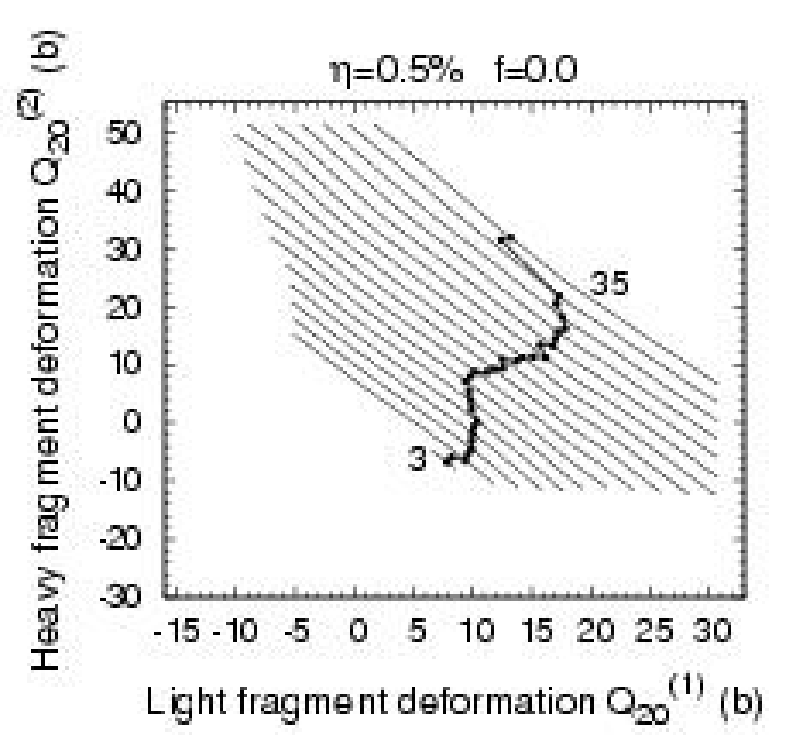
APPLICATION TO $^{252}Cf \longrightarrow {}^{106}Mo + {}^{146}Ba$

FRAGMENT SPIN AS A FUNCTION OF TXE



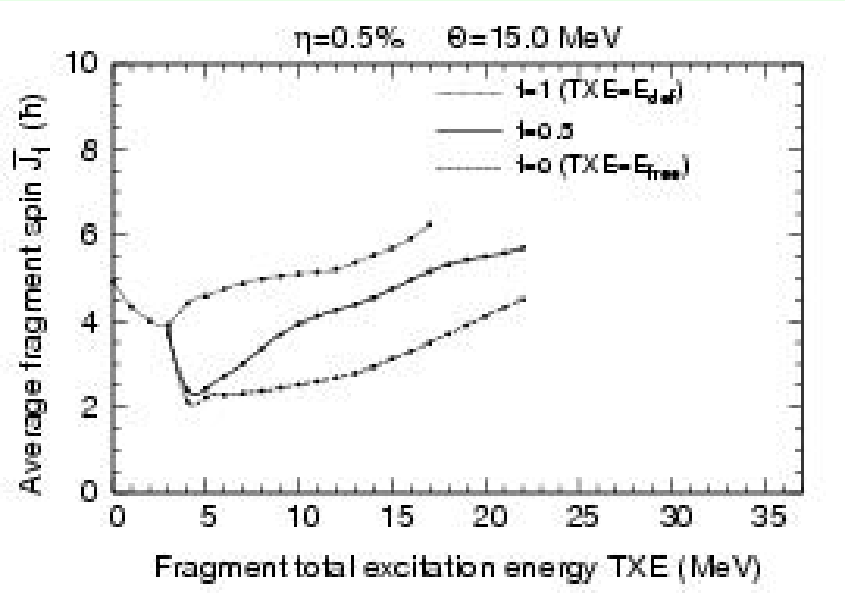
submitted to PRC

TXE contour diagrams



APPLICATION TO $^{252}Cf \longrightarrow {}^{106}Mo + {}^{146}Ba$

FRAGMENT SPIN AS A FUNCTION OF TXE



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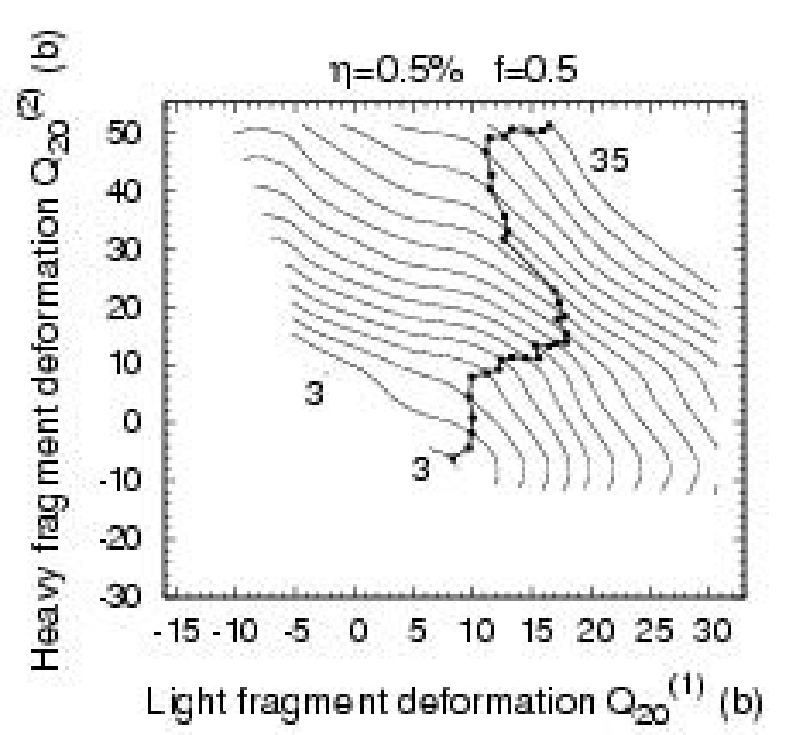
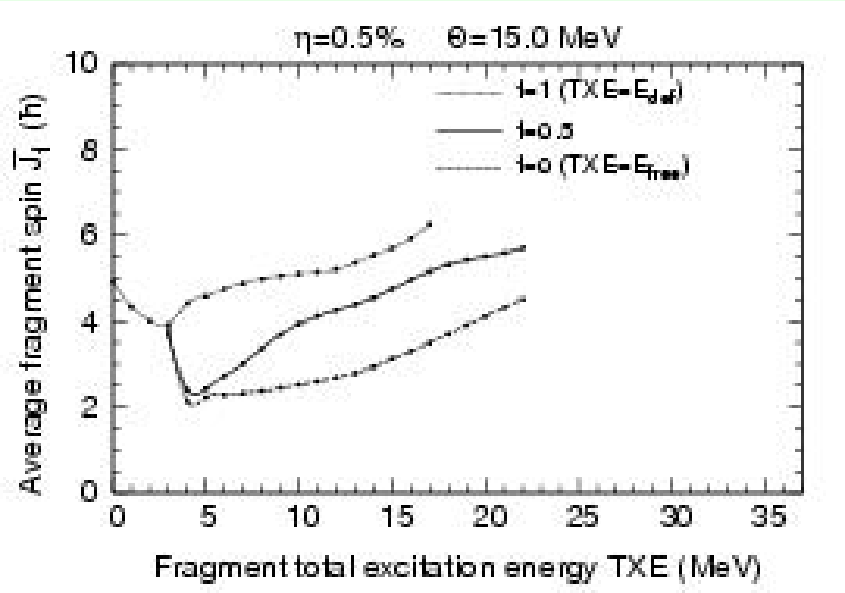


Application to $^{252}Cf \longrightarrow {}^{106}Mo + {}^{146}Ba$

Fragment spin as a function of TXE



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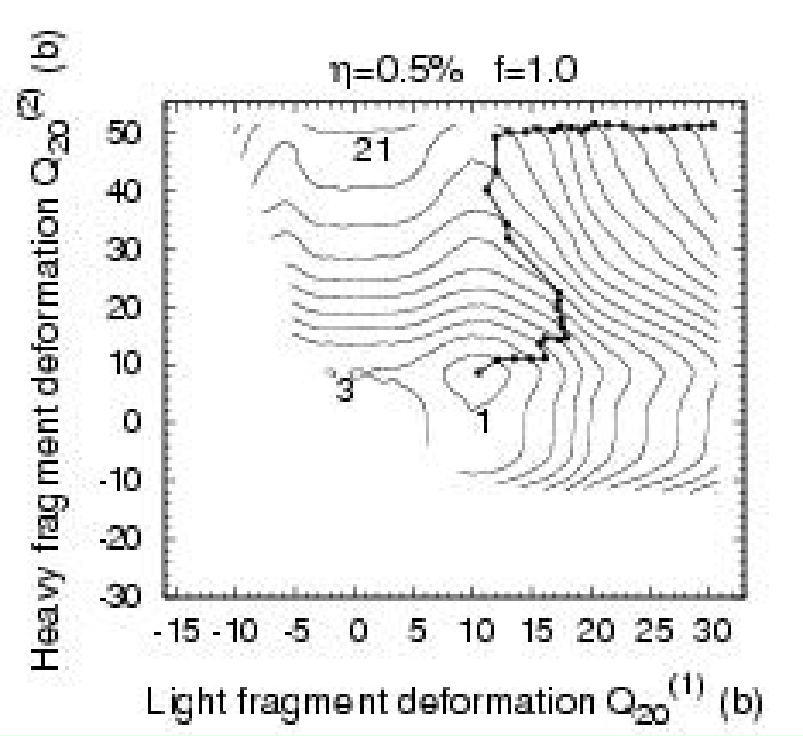

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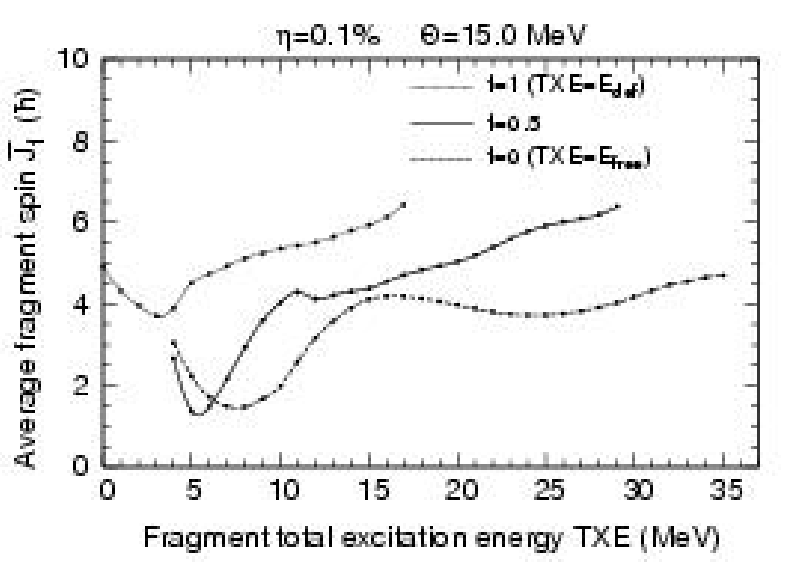
Fragment spin as a function of TXE



smoother variation with $\eta = 0.5\%$ than with $\eta = 0.1\%$