SPY: a microscopic statistical scission-point model to predict fission fragment distributions

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3rd Workshop on Nuclear Density and Gamma Strenght – Oslo, 23-27 May 2011
Fission: an old reaction over towards new challenges

- The fission process is the most complete nuclear physics laboratory
  - Internal nuclear structure (shell effects, pairing,...)
  - Nuclear deformations
  - Dynamics (coupling between collective modes and internal excitation)
- A lot of data and models to interpret them but still...
The scission-point model

- First proposed by Wilkins (Wilkins et al, Phys. Rev. C 14 (1976) 5)
- Static approach:
  - Fission process is slow
  - A statistical «quasi»-equilibrium is reached at scission
  - The main fragment characteristics are freezeed at this point!
  - Dynamics is not explicitly treated
  - The scission configuration is defined by two ellipsoids with an inter-surface distance $d$
The scission-point model

- First proposed by Wilkins (*Wilkins et al, Phys. Rev. C 14 (1976) 5*)
- Static approach
- Based on an energy balance at scission
- Main limitations:
  - Collective and intrinsic temperature parameters (+ d!) fitted on data
  - Energy potentials are relative to the scission point
  - Only prolate deformations
  - Individual energies are not microscopic (liquid drop + Strutinski + pairing)

\[
V(Z_{1,2}, N_{1,2}, \beta_{1,2}, d, \tau_{1,2}) = \Sigma V_{\text{LD}}^{1,2}(Z_{1,2}, N_{1,2}, \beta_{1,2}) + \Sigma V_{\text{Str}}^{1,2}(Z_{1,2}, N_{1,2}, \beta_{1,2}, \tau_{1,2}) + V_{\text{coul}}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) + V_{\text{nucl}}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d)
\]
**The scission-point model: Wilkins**

\[ V(Z_{1,2}, N_{1,2}, \beta_{1,2}, d, \tau_{1,2}) = \Sigma V_{LD}^{1,2}(Z^{1,2}, N^{1,2}, \beta^{1,2}) + \Sigma V_{Str.}^{1,2}(Z^{1,2}, N^{1,2}, \beta^{1,2}, \tau_{1,2}) + V_{coul}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) + V_{nucl}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) \]
The SPY model

- A revised version of Wilkins model was developed by S. Heinrich (PhD thesis, 2006) and J.-L. Sida
- Main core of SPY (Scission Point model for fission fragment Yields)
- Based on microscopic ingredients
  - Individual microscopic energies based on HFB calculation with the Gogny D1S interaction (S. Hilaire, avail. @ Amedee database)
  - No dependence on intrinsic temperature
  - Available energy is calculated as:
    \[ A = E_{\text{tot}} - V \]
    \[ V(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) = \sum V_{\text{HFB}}^{1,2}(Z_{1,2}, N_{1,2}, \beta_{1,2}) + V_{\text{coul}}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) + V_{\text{nucl}}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) \]
- Coulomb interaction based on Cohen Swiatecki formalism
  *Cohen and Swiatecki, Annals of Physics 19 (1962) 67*
- Nuclear interaction based on the Blocki proximity potential
  *Blocki et al, Annals of Physics 105 (1977) 427*
On the scission point definition

- The SPY model is parameter free
- The distance $d$ is fixed at 5 fm
- The distance is chosen on the exit points selection criteria used on Bruyères microscopic fission calculations

Nucleon density at the neck $\rho < 0.01$ fm$^3$
Total binding energy drop ($\approx 15$ MeV)
Hexadecupolar moment drop ($\approx 1/3$)

H. Goutte

238U

23 May 2011
Available energy at scission: asymmetric fragmentation

Driven by the double shell effect of spherical $^{132}\text{Sn}$

$^{104}\text{Mo}$

$^{132}\text{Sn}$

$^{n_{th}} + ^{235}\text{U}$
Available energy at scission: symmetric fragmentation

Quite large deformations available for soft nuclei

Potential Energy Surface for the fragmentation (Z=46, N=72) (Z=46, N=72)

$E_{[MeV]}$

$\beta_2$

$\beta_1$

$n_{th} + ^{235}U$

HFB Energy of the nucleus (Z=46, N=72)

$^{118}\text{Pd}$
The statistical treatment

- The probability of a given fragmentation is linked to the phase space available at scission.
- The phase space is defined by the number of available states of each fragment, i.e. the intrinsic level/state density.
- The energy partition at scission is supposed to be equiprobable between each state available to the system (microcanonical system).
- Therefore the phase space is defined as:

$$\pi(N_l, N_h, Z_l, Z_h, \beta_l, \beta_h, A) = \int_{\varepsilon=0}^{\varepsilon=A} \rho_l(\beta_l, \varepsilon) \rho_h(\beta_h, A - \varepsilon) \, d\varepsilon$$

- The relative probability of a given fragment pair is:

$$P(N_l, N_h, Z_l, Z_h) = \int_0^{\beta_h} \int_0^{\beta_h} \pi(\ldots, \beta_l, \beta_h, A) \, d\beta_l \, d\beta_h$$
The level density ingredient

• Very delicate point of the model...
• In this approach the level densities are a natural counterbalance to a stronger stabilization of spherical deformations and even-even nuclei, which leads to unphysical fragment mass distributions
• For the time being, a Fermi gas approach has been tested
• The CTM effective level density is parameterized as:

\[ \rho_F(E) = \frac{1}{\sqrt{2\pi} \sigma} \frac{\sqrt{\pi}}{12} \frac{e^{2\sqrt{aE}}}{a^{1/4} E^{5/4}} \]

with \( a = \alpha A + \beta A^{2/3} \), \( \alpha = 0.0692559, \beta = 0.282769 \) and \( \sigma = I_0 a \sqrt{E / a} \)
• A microscopic calculation of level densities is actually performed (at zero temperature) in the framework of HFB formalism by S. Hilaire
• Very time consuming since the we need the energy evolution at each deformation for some hundreds of nuclei
From the available energy to the yield

$A_{\text{min}}$

$\eta_{\text{th}} +^{235}\text{U}$

Mass yields

Yields (Log scale)

Yields (Log scale)

Mass yields
Observables: mass and charge yields

\[ n_{th} + ^{235}\text{U} \]

Stefano Panebianco - [SPY: a microscopic statistical scission point model]

CEA – Irfu - SPhN

23 May 2011
Systematics: mass yields for n-induced fission

\[
\begin{align*}
\text{n}_{\text{th}} + ^{229}\text{Th} \\
\text{n}_{\text{th}} + ^{233}\text{U} \\
\text{n}_{\text{th}} + ^{235}\text{U} \\
\text{n}_{\text{th}} + ^{239}\text{Pu} \\
\text{n}_{\text{th}} + ^{245}\text{Cm} \\
\text{n}_{\text{th}} + ^{249}\text{Cf} \\
\text{n}_{\text{th}} + ^{254}\text{Es}
\end{align*}
\]
Systematics: mass yields for spontaneous fission

- $^{246}\text{Cm}(sf)$
- $^{248}\text{Cm}(sf)$
- $^{250}\text{Cf}(sf)$
- $^{252}\text{Cf}(sf)$
- $^{254}\text{Cf}(sf)$
- $^{256}\text{Fm}(sf)$
We miss around 10 MeV: prescission energy (d dependence), Coulomb?
The deformation energy is somehow related to the number of emitted particles.
SPY can already participate to a hot debate...

**β-delayed fission of $^{180}$TI**

Surprising asymmetric yields of $^{180}$Hg fission fully attributed to the nuclear structure of the fissioning nucleus

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Andreyev et al., PRL 105 (2010) 252502
Conclusions and perspectives

• We are developing a statistical scission-point model fully based on microscopic ingredients
• Work in progress but first results are encouraging
• The lack of dynamics is visible (width of yields distributions)
• More work needed on:
  • Coulomb interaction calculation
  • Take into account pre-scission energy into the balance (this can wash out the dependence on $d$)
  • Level density calculations (for “quasi” beginners…)
    • What is the best parametrization?
    • How to parameterize the beta dependence?
    • Is the $E$ dependence really smooth (like Fermi gas)?
    • Microscopic level densities are a useless effort (besides the coherence of the microscopic approach)?
    • Is the spin/parity dependence well under control?
  • Integration of HFB calculation at finite temperature ($E^* \approx T^2$)
  • Integration of full spin populations to calculate isomeric yields
  • …