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

S. Panebianco¹, N. Dubray², H. Goutte¹, S. Heinrich²*, S. Hilaire², J.-F. Lemaître, J.-L. Sida¹

¹CEA Centre de Saclay, Irfu, 91191 Gif-sur-Yvette, France
²CEA, DAM, DIF, 91297 Arpajon, France
* Former member of the laboratory

WONDER 2012
Aix-en-Provence, 25-28 September 2012
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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 freezed at this point
  • Dynamics is not explicitly treated
  • The scission configuration is defined by two ellipsoids with an inter-surface distance $d$

$Z_L, A_L, \beta_L \quad \rightarrow \quad Z_H, A_H, \beta_H$
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)

\[
V(Z_{1,2}, N_{1,2}, \beta_{1,2}, d, \tau_{1,2}) = \sum V_{LD}^{1,2}(Z_{1,2}, N_{1,2}, \beta_{1,2}) + \sum V_{Str.}^{1,2}(Z_{1,2}, N_{1,2}, \beta_{1,2}, \tau_{1,2})
+ V_{coul}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) + V_{nucl}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d)
\]
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 (avail. @ Amedee database)
  - No dependence on intrinsic temperature
  - Available energy is calculated as:
    \[ E_{\text{avail}} = E_{\text{tot}} - V \]
    \[ V(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) = \Sigma V_{\text{HFB}}^{1,2}(Z_{1,2}, N_{1,2}, \beta_{1,2}) + V_{\text{coul}}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) + V_{\text{nucl}}(Z_{1,2}, N_{1,2}, \beta_{1,2}, d) \]
  - 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*
SPY into the Hg fission debate…

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

Andreyev et al., PRL 105 (2011) 252502

Möller et al., PRC 85 (2012) 024306

FIG. 4. (Color online) Minima, saddles, major valleys, and ridges in the 5D potential-energy surface of $^{180}$Hg (see text). At the last plotted point on the fission barrier, $(Q_2/b)^{1/2} \approx 11$, the asymmetry of the shape is $A_H/A_L = 108/72$. 
SPY into the Hg fission debate…

β-delayed fission of $^{180}$Tl

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

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Available energy at scission: symmetric fragmentation

$^{180}\text{Hg fission @ } E^* = 10\text{MeV}$

$^{90}\text{Zr}$
Available energy at scission: asymmetric fragmentation

$^{180}\text{Hg fission @ E}^*=10\text{MeV}$

$^{104}\text{Pd}$

$^{76}\text{Se}$
Available energy at scission

$^{180}\text{Hg fission @ } E^*=10\text{MeV}$
Two reference cases

\[ ^{198}\text{Hg fission @ } E^* = 10 \text{ MeV} \]

\[ ^{236}\text{U fission @ } E^* = 8 \text{ MeV} \]

Iktis et al., Yad. Fiz. 53 (1991) 1225

Stefano Panebianco - [SPY: a microscopic statistical scission point model]
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 $\rho < 0.01 \text{ fm}^3$
Total binding energy drop ($\approx 15 \text{ MeV}$)
Hexadecupolar moment drop ($\approx 1/3$)
On the choice of the scission distance

Self-consistent HFB of $^{180}$Hg:
most probable configuration
$(q_{20}=256.12b ; q_{30}=33.28b^{3/2})$
$d = 5.7$ fm

N. Dubray
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:

\[
P(N_l, N_h, Z_l, Z_h) = \int_0^{\beta_{\text{max}}} \int_0^{\beta_{\text{max}}} \pi(\ldots, \beta_l, \beta_h, A) \, d\beta_l \, d\beta_h
\]
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:

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

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 has been recently performed (at zero temperature) in the framework of HFB formalism
• Very time consuming since the we need the energy evolution at each deformation for some 1500 nuclei
From the available energy to the yield

$^{180}$Hg fission @ $E^*=10\text{MeV}$

$A_{\text{min}}$

Yields

Mass yields
Conclusions and perspectives

- **SPY: a scission-point model fully based on microscopic ingredients (beyond Wilkins)**
- Work in progress but first results are rather encouraging
- Able to **explain the mass asymmetry observed in $^{180}$Hg** fission (paper just submitted for publication…)
- The **lack of dynamics** is visible (width of yields distributions… see B. Jurado talk!) and expected
- Ongoing and future developments (PhD thesis starting):
  - Take into account **pre-scission energy** into the balance (this can wash out the dependence on d)
  - Integration of the new D1M Gogny interaction
  - Integration of HFB calculation at finite temperature ($E^* \approx T^2$)
  - **Microscopic level densities** from HFB (intrinsic + collective)
  - Integration of full spin populations
  - Integration in THALYS
  - …
Backup slides
From the available energy to the yield

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

Minimum of available energy

Yields

Mass yields

Stefano Panebianco - [SPY: a microscopic statistical scission point model]
Observables: mass and charge yields

\( n_{th} + ^{235}\text{U} \)

Ni production yield for \(^{235}\text{U}\) thermal fission

Yield (Log scale)

Z yield

Mass yield

\% of Ni production

Ni fragment mass

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Systematics: mass yields for n-induced fission

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

- $^{246}\text{Cm}(sf)$
- $^{248}\text{Cm}(sf)$
- $^{250}\text{Cf}(sf)$
- $^{252}\text{Cf}(sf)$
- $^{254}\text{Cf}(sf)$
- $^{256}\text{Fm}(sf)$
Systematics: mean TKE

We miss around 10 MeV: prescission energy (d dependence), Coulomb?
Stefano Panebianco - [SPY: a microscopic statistical scission point model]

Systematics: mean deformation energy

The deformation energy is somehow related to the number of emitted particles.
Available energy at scission: asymmetric fragmentation

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

$^{132}$Sn

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

$^{104}$Mo

$^{132}$Sn
Available energy at scission: symmetric fragmentation

Quite large deformations available for soft nuclei

\[ n_{\text{th}} + ^{235}\text{U} \rightarrow ^{118}\text{Pd} \]