

Low-energy fission dynamics

H. Goutte, J.F. Berger and D. Gogny CEA Bruyères-le-Châtel, Lawrence Livermore National Laboratory heloise.goutte@cea.fr

Description of the fission fragment mass distributions

Are the main characteristics of the fragment distributions due to configurations at scission or to the dynamical fission paths followed by the fissionning system ?



Microscopic, quantum-mechanical, time-dependent approach

Assumptions :

- The fission dynamics is governed by the evolution of a few collective parameters q_i
- The internal structure is at equilibrium at each step of the collective motion
- Adiabaticity
- \rightarrow Assumptions valid for low-energy fission (a few MeV above the barrier)

Fission dynamics results from time evolution in collective space Hill-Wheeler wave functions:

 $| \mathbf{h}(\mathbf{u}) \rangle = \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{0} \\ \mathbf{0} \end{bmatrix} \end{bmatrix}$

 $\left|\Psi(t)\right\rangle = \int dq_i f(q_i, t) \left|\Phi_{q_i}\right\rangle$

FORMALISM

Comparison with other possible approaches

 $\left|\Psi(t)\right\rangle = \int dq_i f(q_i, t) \left|\Phi_{q_i}\right\rangle$

- $|\Psi(t)\rangle \neq |\Phi(q(t))\rangle$
- $|\Psi(t)\rangle \neq$ |Slater det er min ant > More correlations than in TDHF
- Explicit time evolution

THEORETICAL METHOD(1)

• Fission dynamics based on Hill-Wheeler wave-function requires two steps :

 $\left|\Psi(t)\right\rangle = \int dq_i f(q_i, t) \left|\Phi_{q_i}\right\rangle$

1- STATICS : determination of the $|\Phi_{q_i}\rangle$

→ Analysis of the properties of the nucleus with respect to different kinds of deformation

Tool : Constrained Hartree-Fock-Bogoliubov method

J.F. Berger *et al.*, Nucl. Phys. A428 (1984) 23c J.F. Berger M. Girod and D. Gogny, Comp. Phys. Comm. 63 (1991) 365.

FORMALISM

THEORETICAL METHOD(2)

1- STATICS : Constrained Hartree-Fock-Bogoliubov method

 $\delta \! \left\langle \Phi_{q_i} \left| \hat{H} - \sum_i \lambda_i \hat{Q}_i - \lambda_N \hat{N} - \lambda_Z \hat{Z} \right| \Phi_{q_i} \right\rangle \! = \! 0 \text{ with the constraints}$

$$\left(\left\langle \Phi_{q_i} \left| \hat{\mathbf{N}}(\hat{Z}) \right| \Phi_{q_i} \right\rangle = \mathbf{N} \left(Z \right) \right)$$

$$\left(\left\langle \Phi_{q_i} \left| \hat{\mathbf{Q}}_i \right| \Phi_{q_i} \right\rangle = q_i \right)$$

2- DYNAMICS : Time-dependent Generator Coordinate Method

 $\frac{\partial}{\partial f^*(q_i,t)} \int_{t_i}^{t_2} \langle \psi(t) | \hat{H} - i\hbar \frac{\partial}{\partial t} | \psi(t) \rangle dt = 0 \qquad \text{with the same } \hat{H} \text{ as in constrained HFB}$

Using the Gaussian Overlap Approximation it leads to a Schroedinger-like equation :

$$H_{\text{coll}}g(t) = i\hbar \frac{\partial g(t)}{\partial t}$$

with

$$H_{coll} = -\frac{\hbar^2}{2} \sum_{i,j} \frac{\partial}{\partial q_i} \frac{1}{M_{ij}(q)} \frac{\partial}{\partial q_j} + \left\langle \Phi_{q_i} \left| \hat{H} \right| \Phi_{q_i} \right\rangle - \sum_{i,j} ZPE_{ij}(q)$$

 \rightarrow Within this method the collective Hamiltonian is entirely determined from microscopic calculations.

Formalism

Static part

1) Use of the D1S Gogny effective interaction

2) Constraints on:

elongation (quadrupole moment \hat{Q}_{20}) asymmetry (octupole moment \hat{Q}_{30}) + (center of mass position (dipole moment \hat{Q}_{10}))

3) Inertia tensor and ZPE calculated using ATDHF approach + Inglis Belyaev approximation

Formalism

Technical points for the dynamical part

1) Discretization on a grid

(Preservation of the hermitian character of the discretized kinetic energy operator)

2) Time-evolution solved using the Crank-Nicholson method (unitary and stable algorithm)

3) Introduction of an imaginary potential at the edge of the box to avoid unphysical reflections

(function of Woods Saxon structure)

POTENTIAL ENERGY SURFACE



Valley landscape:

- ✓ asymmetric valley
- ✓ symmetric valley

PAIRING CORRELATIONS

1) Pairing energy



- No conservation of superfluidity
- Asymmetric valley $E_p \sim 3 \text{ MeV}$ symmetric valley $E_p \sim 15 \text{MeV}$
- → Inertia can be twice as large for a given elongation
 - \rightarrow Important in the dynamical evolution



•The proton gap at the top of the barrier $2\Delta = 2.3$ MeV in good agreement with experimental data*

*F. Vives et al. Nucl. Phys. A662 (2000) 63 -92.

SCISSION LINE AND FRAGMENTS PROPERTIES

- The set of exit points defined for all q_{30} represents the scission line.
- Along the scission line we determine (as functions of q_{30}) :
 - masses and charges of the fragments,
 - the distance between the fragments,
 - the deformation of the fragments,
 - ▶ . . .
- \rightarrow Calculation of :
 - total kinetic energy distribution,
 - static mass and charge distributions,
 - deformation energy of the fragments,
 - ► N/Z ratios of the fragments,
 - ▶ . . .

TOTAL KINETIC ENERGY

TKE (A_H)
$$\approx \frac{Z_H Z_L e^2}{d(A_H)}$$

• The dip at $A_H = A_L$ and peak at $A_H \approx 134$ are well reproduced

• Overestimation of the structure (up to 6% for the most probable fragmentation)



FRAGMENT MASS DISTRIBUTION FROM 1D MODEL

Vibrations along the scission line







FRAGMENT MASS DISTRIBUTION FROM 1D MODEL

$$Y(A_{\rm H}, A_{\rm L}) = \left|\Psi_0^{+1}(q_{30})\right|^2$$



- Maxima are well located
- Widths are 2 times smaller

DYNAMICAL RESULTS

Time evolution from ground state to exit points "Dynamical" distribution: from the flux of the w.f. passing through scission line



CONSTRUCTION OF THE INITIAL STATE

Determination of the initial state :

Quasi-stationnary states of the modified 2D first well



- Only states with B_f ≤ E ≤ 2 MeV have been considered (~ 14 states)
 → the adiabatic assumption is justified
- Initial states are eigenstates of the parity with a +1 or –1 parity.

• What is the influence of the nodal structure of the initial states on the mass distribution ?

DYNAMICAL RESULTS INFLUENCE OF THE INITIAL STATE

- Small effects on the widths and locations of the maxima
- Peak-to-valley ratio (R) much sensitive to the parity of the initial state
 - ▶ positive parity state R ~50
 - negative parity state R ~ infinity
 - ▶ experimental results R ~ 100



The parity content of the initial state controls the symmetric fragmentation yield.

DYNAMICAL RESULTS INITIAL STATES FOR THE ²³⁷U (n,f) REACTION(1)

• Percentages of positive and negative parity states in the initial state in the fission channel

$$p^{-}(E) = \frac{\sigma(\pi = -1, E)}{\sigma(\pi = -1, E) + \sigma(\pi = +1, E)}$$
$$p^{+}(E) = \frac{\sigma(\pi = +1, E)}{\sigma(\pi = -1, E) + \sigma(\pi = +1, E)}$$

with E the energy and $P = \pi (-1)^{I}$ the parity of the compound nucleus (CN)

$$\sigma(\pi = -1, E) = \sum_{I=2p, P=-1}^{\infty} \sigma_{CN}(P, I, E) P_f(P, I, E) + \sum_{I=2p+1, P=+1}^{\infty} \sigma_{CN}(P, I, E) P_f(P, I, E)$$

$$\sigma(\pi = +1, E) = \sum_{I=2p, P=+1}^{\infty} \sigma_{CN}(P, I, E) P_f(P, I, E) + \sum_{I=2p+1, P=-1}^{\infty} \sigma_{CN}(P, I, E) P_f(P, I, E)$$

where σ_{CN} is the formation cross-section and P_f is the fission probability of the CN that are described by the Hauser – Feschbach theory and the statistical model.

INITIAL STATES FOR THE ²³⁷U (n,f) REACTION (2)

• Percentage of positive and negative parity levels in the initial state as functions of the excess of energy above the first barrier

E(MeV)	1.1	2.4
P+(E)%	77	54
P⁻(E)%	23	46

W. Younes and H.C. Britt, Phys. Rev C67 (2003) 024610.

LARGE VARIATIONS AS FUNCTION OF THE ENERGY Low energy : structure effects High energy: same contribution of positive and negative levels

DYNAMICAL RESULTS EFFECTS OF THE INITIAL STATES



DYNAMICAL RESULTS DYNAMICAL EFFECTS ON MASS DISTRIBUTION

Comparisons between 1D and « dynamical » distributions

- Same location of the maxima
 → Due to properties of the potential energy surface (well-known shell effects)
- Spreading of the peak
 → Due to dynamical effects :
 (interaction between the 2 collective modes via potential energy surface and tensor of inertia)
- Good agreement with experiment



H.Goutte et al. Nucl. Phys. A734 (2004) 217 H. Goutte, J.-F. Berger, P. Casoli and D. Gogny Phys. Rev. C71 (2005) 024316

CONCLUSIONS

- First microscopic quantum-dynamical study of fission fragment mass distributions based on a time-evolution formalism.
- Application to ²³⁸U: good agreement with experimental data.

- Most probable fragmentation due to potential energy surface properties
- Dynamical effects on the widths of the mass distributions, and influence of the initial condition on the symmetric fission yield have been highlighted.