(A)symmetry of Fission in the

\[ 74 \leq Z \leq 90, \ A \leq 205 \]

Region.

P. Möller (LANL) and J. Randrup (LBL)

Collaborators on this and other projects: W. D. Myers, H. Sagawa (Aizu), S. Yoshida (Hosei), T. Ichikawa (YITP), A. J. Sierk (LANL), A. Iwamoto (JAEA), S. Aberg (Lund), R. Bengtsson (Lund), S. Gupta (IIT, Ropar), and many experimental groups (e. g. K.-L. Kratz (Mainz), H. Schatz (MSU), A. Andreyev (University of West Scotland), . . . )

More details, figure files, papers, data on

http://t2.lanl.gov/molleretal

This is our new web site! The previous “private” one maintained locally was killed after more than 15 years in existence. The new one is officially managed by our laboratory computer people, although we program all the web pages (mostly by me).
THEMES

My presentation will have 4 themes:

• To calculate yields accurate potential-energy surfaces are absolutely necessary

• Accuracy includes height of saddles and ridges as well as their location in a high-dimensional space

• Benchmarking of yield model on nuclei from Th to Fm.

• Application to neutron-deficient Hg region.
Mass Models Compared to AME2003

FRLDM(2002):  
\( \sigma = 0.72 \) (MeV)  
\( \mu = -0.03 \) (MeV)

HFB(Sly4):  
\( \sigma = 5.11 \) (MeV)  
\( \mu = -2.94 \) (MeV)

\( M_{\text{exp}} - M_{\text{th}} \) (MeV)

Neutron Number \( N \)
$\sigma = 7.33 \text{ (MeV)}$

$\mu = -3.93 \text{ (MeV)}$
Effect of Axial Asymmetry on Nuclear Mass

![Graph showing the effect of axial asymmetry on nuclear mass with neutrons and protons plotted on the x and y axes respectively. The graph includes various isotopes and energy levels indicated on the plot.]
Mass-model error without $\gamma$ correction for 71 nuclei with $|\Delta E_\gamma| > 0.2$ MeV

$\sigma = 0.577$ MeV
$\mu = -0.452$ MeV

Mass-model error without $\varepsilon_3$ correction for 78 nuclei with $|\Delta E_{\varepsilon_3}| > 0.2$ MeV

$\sigma = 1.160$ MeV
$\mu = -1.032$ MeV

Mass-model error with $\gamma$ correction for 71 nuclei with $|\Delta E_\gamma| > 0.2$ MeV

$\sigma = 0.381$ MeV
$\mu = -0.109$ MeV

Mass-model error with $\varepsilon_3$ correction for 78 nuclei with $|\Delta E_{\varepsilon_3}| > 0.2$ MeV

$\sigma = 0.385$ MeV
$\mu = -0.168$ MeV
New Masses in Audi 2003 Evaluation, Relative to 1989, Compared to Theory

FRLDM (1992)

$\sigma_{1654} = 0.779$ MeV
$\sigma_{529} = 0.685$ MeV

FRDM (1992)

$\sigma_{1654} = 0.669$ MeV
$\sigma_{529} = 0.462$ MeV
$\alpha$-decay of $^{278}\text{113}$

- **RIKEN exp. (2004)**
- **OTHER exp.**
- **FRDM (1992)**
- **FRLDM (1992)**
- **HFB8 (Goriely)**
- **HFB2 (Goriely)**

Neutron Number $N$

153  155  157  159  161  163  165  167

Proton Number $Z$

101  103  105  107  109  111  113  115

Energy Release $Q_{\alpha}$ (MeV)
Scale 1.00 (MeV)

Spheroidal Deformation $\varepsilon_2$
Distance between Mass Centers $r$ (Units of $R_0$)

Fragment Elongation $\sigma$ (Units of $R_0$)

Family of shapes considered
Potential energy for $^{258}$Fm

Distance between Mass Centers $r$ (Units of $R_0$)

Fragment Elongation $\sigma$ (Units of $R_0$)

$E$ (MeV)
Dam building flips waterflow across new saddle

Imaginary Water-Flow Strategies

Energy: $E(I,J,K,L,N)$
Wetness: $IW(I,J,K,L,N)$ (Wet=1, Dry=0)

Retaining wall prevents backflow
One-Dimensional Paths

Saddle point

Function Value

θ
Numerical search of discontinuities in self-consistent potential energy surfaces

N. Dubray\textsuperscript{a}, D. Regnier\textsuperscript{b}

\textsuperscript{a}CEA, DAM, DIF, F-91297 Arpajon, France
\textsuperscript{b}CEA, DEN, DER, F-13108 Saint Paul les Durance, France

Abstract
Potential energy surfaces calculated with self-consistent mean-field methods are a very powerful tool, since their solutions are global minima of the non-constrained subspace. However, this minimization leads to an incertitude concerning the saddle points, that can sometimes be no more saddle points in bigger constrained subspaces (fake saddle points), or can be missing on a trajectory (missing saddle points). These phenomena are the consequences of discontinuities of the self-consistent potential energy surfaces (SPES). These discontinuities may have important consequences, since they can for example hide the real height of an energy barrier, and avoid any use of a SPES for further dynamical calculations, barrier penetrability estimations, or trajectory predictions. Discontinuities are not related to the quality of the production of a SPES, since even a perfectly converged SPES with an ideally fine mesh can be discontinuous. In this paper we explain what are the discontinuities, their consequences, and their origins. We then propose a numerical method to detect and identify discontinuities on a given SPES, and finally we discuss what are the best ways to transform a discontinuous SPES into a continuous one.

Keywords: self-consistent methods, potential energy surfaces, total binding energy, HFB

Introduction

Potential energy surfaces (PES) are a widely used tool to describe physical and chemical systems, among others. Numerous methods exist to extract from a PES local minima, saddle points, and least energy paths between local minima [1, 2]. To produce a PES, a method giving the energy of a system as a function of a given number of constrained variables is needed. In this paper, we will separate these methods into two main classes: self-consistent and non-self-consistent methods. Surfaces associated with these methods will be called Self-consistent Potential Energy Surfaces (SPES) and Non Self-consistent Energy Surfaces (NSPES), respectively. In nuclear physics, SPES can be obtained for example by constrained Hartree-Fock methods and extensions [3, 4, 5, 6], by constrained Relativistic Mean Field method [7], etc. . . NSPES can be produced by several methods, ranging from the historical liquid drop model [8, 9] to the well-known macroscopic-microscopic model, using parametrization of the nuclear mean-field deformation [10, 11].
Five Essential Fission Shape Coordinates

\[ Q_2 \sim \text{Elongation (fission direction)} \]
\[ \alpha_g \sim \frac{(M1-M2)}{(M1+M2)} \text{ Mass asymmetry} \]
\[ \varepsilon_{f1} \sim \text{Left fragment deformation} \]
\[ \varepsilon_{f2} \sim \text{Right fragment deformation} \]
\[ d \sim \text{Neck} \]

\[ \Rightarrow \ 5\ 315\ 625 \text{ grid points} - 306\ 300 \text{ unphysical points} \]
\[ \Rightarrow \ 5\ 009\ 325 \text{ physical grid points} \]
Figure 37

$^{252}\text{Fm}$

Distance between Mass Centers $r$ (Units of $R_0$)

Nuclear Inertia $B_r$ (Units of $\mu$)

- Cranking (dynamic)
- Cranking (static)
- Semi-empirical
- Irrotational
- Reduced mass $\mu$
do not necessarily lead to identical half-lives for each individual nucleus. Rather, each set leads to a best overall reproduction of the experimental half-life data.\textsuperscript{23}

IV. RESULTS AND DISCUSSION

A. The experimentally known region

With the fission barrier potentials established as described in Sec. II we have, using the different sets of trial inertial-mass functions described in Sec. III calculated the spontaneous-fission half-lives for the known even-even nuclei ranging from $^{232}$U to $^{258}$No. (The theoretical deformation energies for the known isotopes of element 104 are not very accurate and we have excluded this element from the test group. This exclusion should also be seen in the light of the present disagreement between reported half-lives for isotopes of this element.) Minimization of the average logarithmic deviation $\Delta$ of the calculated half-lives from the experimental ones determines, for each set of inertial functions, the adjustable parameter(s) entering the trial functions. (For collection of recent half-life data see Refs. 23–25.)

1. Macroscopic inerti

For the hydrodynamic-type inertial-mass function with $c = 1$ the best reproduction of experimental half-lives is obtained for $k = 11.5$. This value is larger than the previously\textsuperscript{26} employed value of 10.0 This change is mainly due to the inclusion of the $\xi_4$ dependence of the $r$ coordinate; cf. our discussion of this point in Sec. II. The average logarithmic deviation is $\Delta = 1.7$, which corresponds to a factor of around 50.

In Fig. 4 the solid curves indicate these effective mass functions. The half-lives obtained with this set of effective mass functions are shown in Fig. 5, together with the experimental data.

In agreement with the results of our earlier study\textsuperscript{8} based on an older set of barriers, it turns out that a simultaneous variation of the slope parameter $c$ appearing in the inertial-mass function leads to a better fit. In a contour plot of the quantity $\Delta$ as a function of $k$ and $c$ there is a valley passing approximately through the points $(k = 11.5, c = 1.0)$ and $(k = 6.5, c = 0.5)$. The variation of $\Delta$ in the direction perpendicular to the valley is rapid while along the valley the slope is rather gentle. The absolute minimum is located around $(k = 6.5,$

![Diagram](image)

FIG. 4. Effective fission inertial-mass functions for the same four nuclei as in Fig. 3. The solid smooth curve $(k = 11.5, c = 1.0)$ is the best macroscopic inertial function with $c$ fixed to unity. The dashed curve $(k = 11.5, c = 0.5)$ results (approximately) if $c$ is also allowed to vary in the fit. The best microscopic inertial-mass function has $\rho = 0.80$ and is indicated by the solid wiggly curve.

![Diagram](image)

FIG. 5. Spontaneous-fission half-lives calculated with the macroscopic inertial-mass functions having $k = 11.5$ and $c = 1.0$ (open circles joined by dashed lines). The experimental values are indicated by solid squares joined by solid lines. In the lower left corner are included the square brackets in which various isomeric half-lives. Also included in the figure are the half-lives calculated with the estimated approximate barriers for the transuranium elements (dots joined by dotted lines).
Fission Barrier and Associated Shapes for $^{228}\text{Ra}$

- Symmetric mode
- Asymmetric mode
- Separating ridge

Potential Energy (MeV) vs. Nuclear Deformation ($Q_2/b^{(1/2)}$)
Triple No of Elongation Grid Points: 133 Points in $Q_2$ in all Panels

- **$^{233}$Pu(n,f) Calc.**
- **$^{235}$Pu(n,f) Calc.**
- **$^{236}$U Calc.**
- **$^{234}$U(n,f) Calc.**
- **$^{234}$U(γ,f) Exp.**

Yield $Y(Z_f)$ (%)

Fragment Charge Number $Z_f$

30 40 50 60
\( Fm_{255} \) and \( Fm_{256} \) mass yield as a function of charge number \( Z \). The graph shows a peak at \( Z \approx 50 \) with a broad distribution, indicated by the black circle and the dashed line for the experimental data of \( \text{Exp. } ^{255}\text{Fm}(n,f) \).
Fragment mass number $A_f$ vs. Yield $Y(A_f)\%$ for $^{256}\text{Fm}$.

- **Calc. (6.38 MeV)**
- **Exp. $^{255}\text{Fm}(n,f)$**
5D Brownian motion

$Fm(n,f)$

Calc. (7 MeV)

Fragment Mass Number $A_f$

Yield $Y(A_f)$ (%)

$R_{sc}=1.5$ fm

$Fm_{(n,f)}$ Calc. (7 MeV)

5D Brownian motion

$2^{60}Fm$

$2^{58}Fm$

$2^{257}Fm(n,f)$

$2^{58}Fm$ Calc. (7 MeV)

4D Scission surface

$R_{sc}=1.5$ fm

Fragment Mass Number $A_f$

Yield $Y(A_f)$ (%)
Folded-Yukawa potential

\[ T_{1/2} = 1.74 \text{ (s)} \]

\[ ^{18}_{81}\text{Ti} \rightarrow ^{180}_{80}\text{Hg} + e^+ \]

\[ \varepsilon_2 = -0.130 \quad \Delta_n = 0.99 \text{ MeV} \quad \lambda_n = 34.88 \text{ MeV} \]

\[ \varepsilon_4 = 0.010 \quad \Delta_p = 0.51 \text{ MeV} \quad \lambda_p = 32.50 \text{ MeV} \]

\[ \varepsilon_6 = 0.010 \quad (L-N) \quad a = 0.80 \text{ fm} \]
Asym. Valley
Fission Barrier
Q
EC
Sym. Trough
Ridge

$^{174}$Hg

Potential Energy (MeV)

Nuclear Deformation ($Q_2/b^{1/2}$)
Asym. Valley
Sym. Valley
Fission Barrier
Fission Ridge

$Q_{EC}$

Nuclear Deformation \( (Q^2/b)^{(1/2)} \)

Potential Energy (MeV)

$^{180}\text{Hg}$
Potential Energy (MeV)

Nuclear Deformation \((Q_2/b)^{(1/2)}\)

\(^{188}\text{Hg}\)

Asym. Valley
Sym. Valley
Fission Barrier
Ridge

\(Q_{EC}\)

\(0\ 2\ 4\ 6\ 8\ 10\ 12\)

\(0\ 5\ 10\ 15\ 20\ \)
CONCLUSIONS

• First generation model describes actinide yields from Th to Fm with unexpected (to me) accuracy.

• Hg yields are somewhat more roughly described, but lack of data inhibits precise understanding of deviations, (if any). Most experimental yield is subbarrier. Interesting energy dependence obtained for $^{174}$Hg, symmetric yield increases with decreasing energy.

• Studies of entire isotope chains indicates transition from asymmetric below approximately $A = 200$ to symmetry beyond. Highly variable behavior below Pb.

Future enhancements?:

• What’s beyond “Brownian shape motion?”

• Odd-even effects and ($Z, N$) yields.

• Experimental tests of predictions in region below Pb HIGHLY desirable.
METROPOLIS

The simplicity of the algorithm nobly stands aside the complexity of the problems it successfully treats.