Computational Approaches to Whole Process of Nuclear Fission


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Background and introduction

1. Nuclear fission is the key physics process as a base for generation of energy in nuclear technology
2. Therefore, nuclear data related to nuclear fission is most important
3. Nuclear fission is also important in understanding origin of heavy elements in r-process nucleosynthesis, since fission recycling seems to be occurring on NS-NS merger scenario
4. Due to complexity of the process, nuclear fission still offers a field of big challenges for nuclear physics, especially, the process from compound nucleus to scission is still a mysterious process
Time evolution of fission

複合核の形成
Compound nucleus

サドル点
Saddle, 2nd minima

断裂点
Scission

核分裂片
(Fission Fragment)

1次収率
(Primary Yield)

核データ
Nuclear Data

独立収率
(Independent Yield)

累積収率
(Cumulative Yield)

断裂中性子
Scission neutron

10^{-18} sec.

即発中性子及びγ
Prompt n and γ

(一次)核分裂生成物
(Primary Fission Product)

10^{-16} sec.

β− decay

(二次)核分裂生成物
(Secondary Fission Product)

60 sec.

HF_3D, CoH
FREYA
GEF, P2P
FIFRELYN
TALYS
ABLA, ....

start from here

AMD simulation

核分裂片

独立収率

Cumulative Yield

核データ

Nuclear Data

核分裂生成物

Primary Fission Product

核分裂生成物

Secondary Fission Product

β− decay

β− decay

β− decay

β− decay

β− decay
Systematics of average peak position of light (L) and heavy (H) fragments

\[ \langle A_H \rangle \]

\[ \langle A_L \rangle \]

- JENDL-4.0 FPY 14MeV Best Fit
- JENDL-4.0 FPY 14MeV
- Microscopic Calc.
- Macroscopic Calc.
Systematics and anomaly in the average Total Kinetic Energy of Fission Fragments
Multiplicity distributions of prompt neutrons and its dependence on excitation energy
Multiplicity distributions of prompt neutrons and its dependence on excitation energy

Why does it have saw-tooth structure like this? Why only neutron multiplicity of the heavy fragments increases? Entropy sorting??? Need for interpretation from dynamical theory
Charge polarization and fine structure of FPY by Wahl

\[ \Delta Z = Z_{FF}(A_{FF}) - \frac{Z_c}{A_c} A_{FF} \]

Is this behavior real?
Our recent microscopic calculation denies it
6. Many observables arise as a result of fission, e.g., fission fragment yield, TKE, population of prompt neutrons and gammas which is followed by a series of $\beta$–decay and associated delayed processes, and they must be comprehended in a consistent manner, which is still a formidable task.

7. These quantities, either as a single physics quantity or their correlations, have been treated in a phenomenological way in the past.

8. We have been treating the process before scission by several theories, such as Langevin model, AMD and TDHF, and their outcomes are connected to statistical decay model HF$_3$D (presentation by S. Okumura) and Gross theory of $\beta$–decay (mostly by T. Yoshida).

9. In this presentation, I concentrate on the process from compound nucleus to the instance of scission, and try to elucidate origin of systematic and anomalous trends in fission observables and their correlations by our 4–dimensional Langevin calculation (a macro–micro approach).
Simulation of nuclear fission ($^{235}$U + 140 MeV n) by JQMD

$\begin{align*}
\text{JQMD} : \text{JAERI Quantum Molecular Dynamics} \\
= \text{a semiclassical molecular dynamics for nuclear reactions (mean field + NN collision)}
\end{align*}$
Simulation of nuclear fission \((^{235}\text{U} + 140 \text{ MeV n})\) by JQMD

\[
t = 0 \text{ fm/c}
\]

Time evolution of \(^{235}\text{U} + 140 \text{ MeV n}\) reaction by JQMD

Nuclear fission by Langevin equation

Nuclear shape evolution is driven by random kicks by nucleons in thermal equilibrium (microscopic d.o.f.) given to the nuclear surface (macroscopic d.o.f) from inside the surface.

These 2 different d.o.f have different time scales:

• nucleon motion : 1 to 10 fm/c
• shape motion : $\sim >10,000$ fm/c
4D Langevin model of fission

\[
\begin{align*}
\frac{dq_i}{dt} &= \left(m^{-1}\right)_{ij} p_j \\
\frac{dp_i}{dt} &= -\frac{\partial F}{\partial q_i} - \frac{1}{2} \frac{\partial}{\partial q_i} \left(m^{-1}\right)_{jk} p_j p_k - \gamma_{ij} \left(m^{-1}\right)_{jk} p_k + g_{ij} R_j(t)
\end{align*}
\]

\{q_i : i = 1..4\} = \{Z, Z_0, \alpha, \delta_L, \delta_R\}

\(F\): Helmholtz’ free energy, \(F = E - TS\)

\(q_i\): Nuclear shape motion

\(p_i\): Momentum conjugate to \(q_i\)

\(m_{ij}\): Inertia tensor

\(\gamma_{ij}\): friction tensor

\(g_{ij}g_{ij} = \gamma_{ij}T\) : Fluctuation dissipation theorem (+Einstein relation)

\[
T = \sqrt{\frac{E^* - \frac{1}{2} m_{ij} p_i p_j - E_{rot}}{\alpha}}
\]

\(E^*\): Total excitation energy of the system

C. Ishizuka et al., PRC 96, 064616 (2017).
Shape parametrization

Two-center model
(Maruhn and Greiner, Z. Phys. 251(1972) 431)

Collective coordinates (3 or 4 dynamical variables)

\[ \{q\}_{3D} = \{ZZ_0, \delta, \alpha\} \quad \{q\}_{4D} = \{ZZ_0, \delta_1, \delta_2, \alpha\} \]

- \( ZZ_0 = \frac{z_0}{R} \) \quad \text{Elongation} \quad R : \text{Radius of compound nucleus} = 1.2 \frac{A_{CN}^{1/3}}{}
- \( \delta_i = \frac{3(a_i - b_i)}{2a_i + b_i} \) \quad \text{Deformation of fragments} \quad 3D : \delta_1 = \delta_2 = \delta \quad 4D : \delta_1, \delta_2 \text{ are independent}
- \( \alpha = \frac{A_1 - A_2}{A_1 + A_2} \) \quad \text{Mass asymmetry} \quad A_1 : \text{mass of the right fragment} \quad A_2 : \text{mass of the left fragment}
- \( \varepsilon = 0.35 \) \quad \text{neck parameter : fixed} \quad \text{volume conservation condition is applied}
Predictions for mass distributions (Ex=20MeV)
Mass–TKE correlation and its decomposition

$^{236}\text{U} (n_{th}+^{235}\text{U})$

$^{258}\text{Fm}(B_f+2\text{MeV})$

Super Long

Super Short

Q-value

TKE (MeV)

A (u)

Mass, A
Systematics in Mass–TKE correlations

U236 to Fm256

Neck parameter, $\epsilon = 0.35$
Systematics in Mass–TKE correlations

From Fm257 to Lr259

Neck parameter, $\epsilon = 0.35$
Results of mass–TKE correlations

TKE Systematics: fission mode components

(ε=0.35)
Estimation of excitation energy of fragments: important input to subsequent statistical-decay calculation

1. Estimation from TKE (Langevin) and Q-value

\[ TXE = EX(A_L) + EX(A_H) = Q - TKE \]

\[ EX(A_{FF}) = a(A_{FF})T(A_{FF})^2 + \text{correction}(A_{FF}) \]

\[ \frac{T_L}{T_H} \approx 1.3, \text{ or } f(A_{FF}) \]

2. Direct estimation from Langevin result

\[ EX(A_{FF}) = E_{\text{def}}(A_{FF}) + E_{\text{vib}}(A_{FF}) + a(A_{FF})T_{\text{Langevin}}^2 + E_{\text{rot}} \]

\[ = f(\delta(A_{FF})) = K.E. \text{ of } \delta(A_{FF}) = \text{Intrinsic Energy} \]

→ presentation by Shin Okumura
Clear correlation of fragment deformation and saw-tooth structure of prompt neutron multiplicity
Correlation of energy dependence of fragment deformation and saw-tooth structure of prompt neutron multiplicity
Reactor Antineutrino Energy Spectra; Comparison Between the Current Prediction Basis (ILL) and Gross Theory Calculation

T. Yoshida et al., PRC (in press)

Decay heat
Delayed neutrons
Concluding remarks

• We are constructing a computational framework to cover the whole process of fission, starting from compound nucleus, scission, prompt particle emission and $\beta$-decay.
• I covered the first part of the fission process, namely, from the compound nucleus to saddle to scission, based on our 4D Langevin approach, which gives the initial conditions to following statistical decay calculations
• The 4D Langevin can explain nicely a systematical and anomalous trends in mass distribution, TKE and their correlation
• Our approach can give reasonable distribution for deformation of fragments, from which we can estimate excitation energy of fission fragments, although the process is still under development
• A microscopic approach to charge polarization is on going (tbs)
• Connection to SHE studies is promising
• Successive statistical decay will be a subject of S. Okumura’s talk
Thank you very much