Microscopic Neutron Emission and Fission Rates in Compound Nuclei

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Collaborations:

F.R. Xu, W. Nazarewicz, G. Fann, M. Kortelainen, P. Schuck,
Y. Zhu, Y.N. Zhang, X.Y. Xiong, K. Wang, N. Fei, …..
And many others for discussions

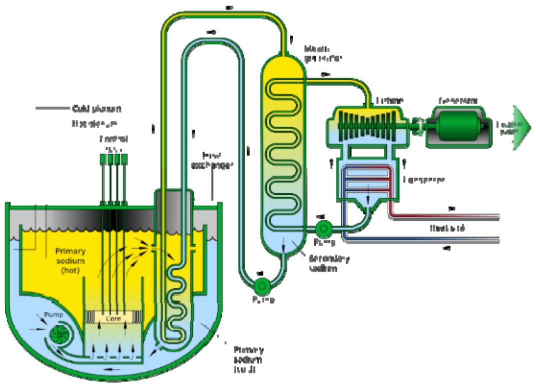
- Yi Zhu and J.C. Pei, Phys. Rev. C 90, 054316(2014).
- Yi Zhu and J.C. Pei, Phys. Rev. C 94, 024329(2016).

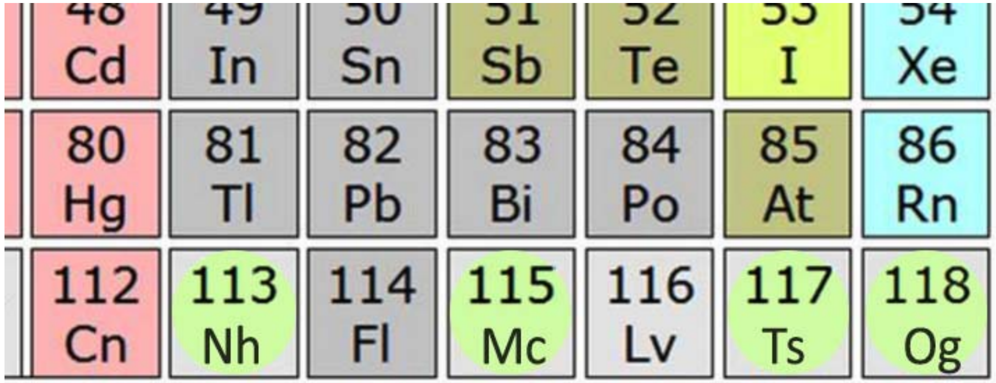
SSNET Workshop, 2016.11, Gif sur Yvette, France

Contents

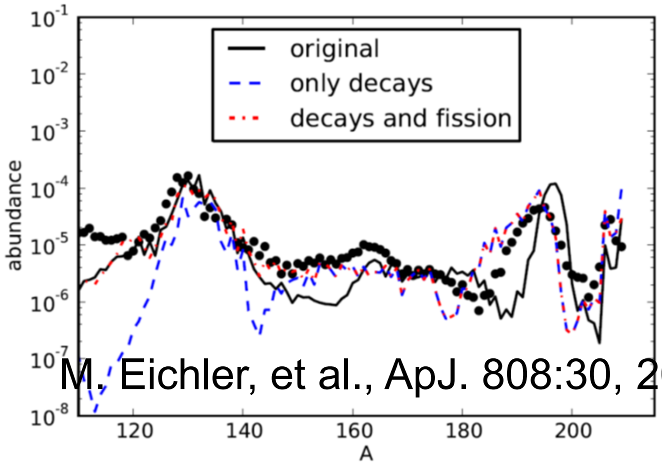
Motivation

Practical Interests: fast-neutron induced fission in reactors, fission in astrophysical environments, synthesis of superheavy nuclei……





4 new elements named by IUPAC/IUPAP



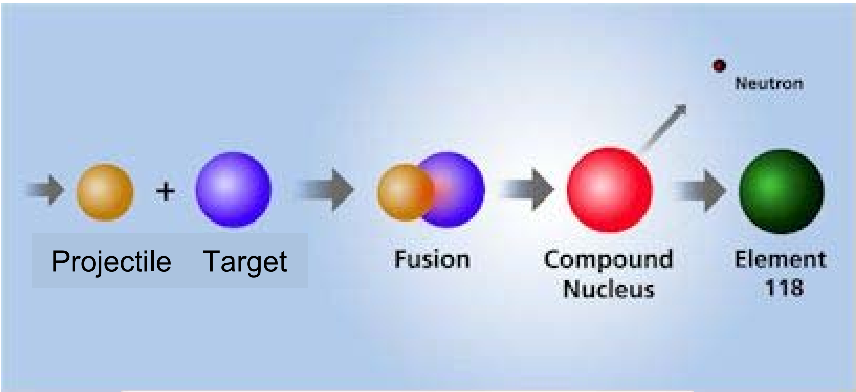
M. Eichler, et al., ApJ. 808:30, 2015

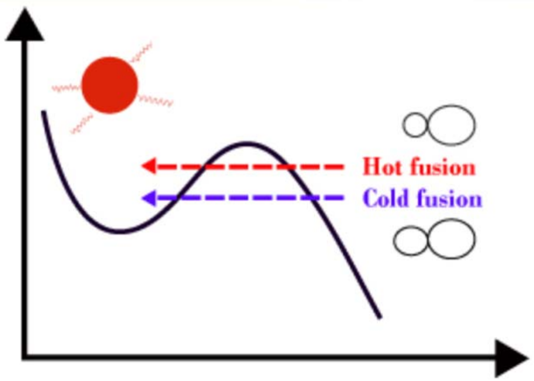
fission in neutron start merger affect r-process abundance

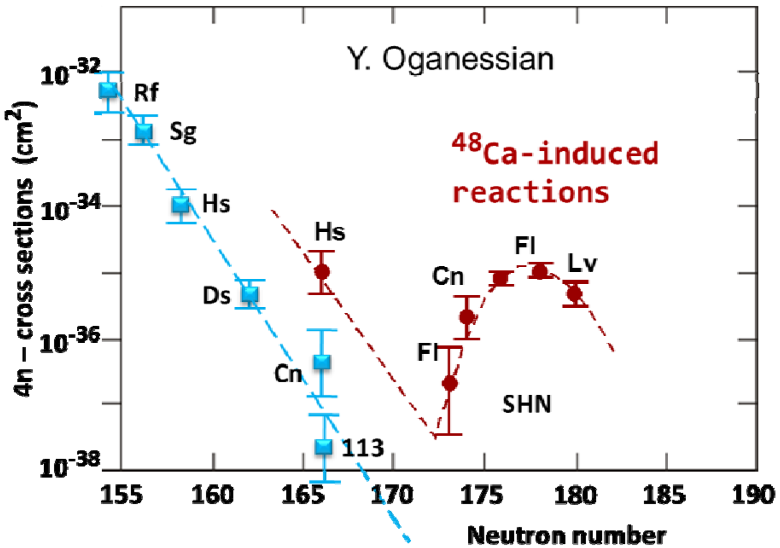
Introduction

- The competition between neutron emission and fission is crucial for the survival probabilities of compound SHN.
- It is particularly an interesting issue for hot-fusion reactions

$$\boxed{\sigma_s(E_{\mathrm{c.m.}}) = \sigma_{cap}^{eff}(E_{\mathrm{c.m.}}) P_{CN}(E_{\mathrm{c.m.}}) W_s(E_{\mathrm{c.m.}})}$$







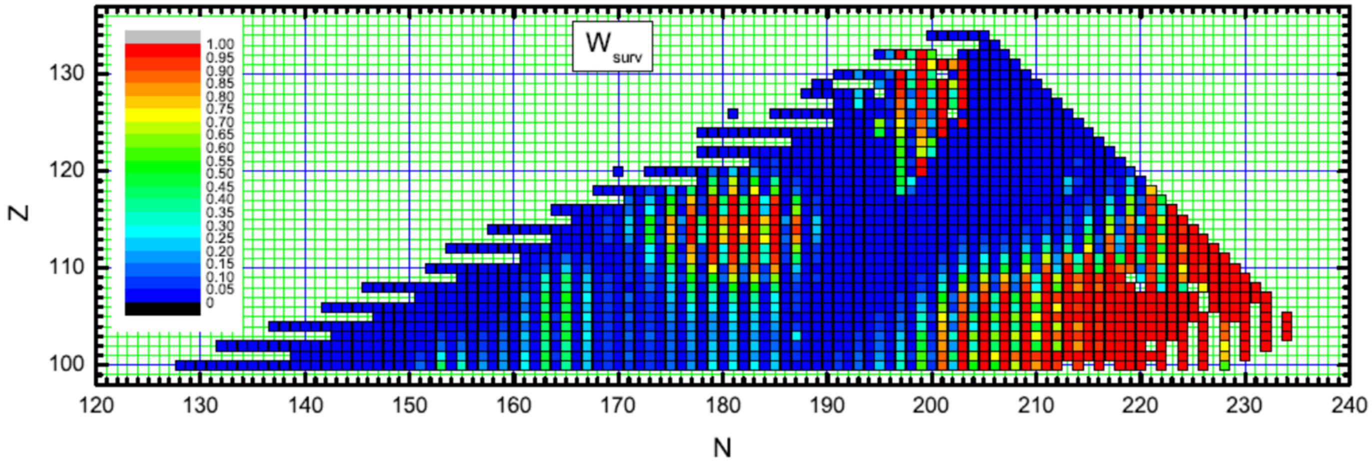
Very large cross sections for hot fusion

the surprise N=176

- The calculations of survival probabilities are usually based on Bohr-Wheeler statistical model

$$\Gamma_{\rm n}(E^*, J) = \frac{2m_{\rm n}R^2}{\pi\hbar^2} \int_0^{E^*-S_{\rm n}} \frac{\rho(E^*-S_{\rm n}-\varepsilon_{\rm n}, J)}{\rho(E^*, J)} \varepsilon_{\rm n} d\varepsilon_{\rm n}$$

$$\Gamma_{\rm f}(E^*, J) = \frac{1}{2\pi} \int_0^{E^*-B_{\rm f}} \frac{\rho_{\rm s.d.}(E^*-B_{\rm f}-\varepsilon_{\rm f}, J)}{\rho_{\rm s.d.}(E^*, J)} T_{\rm f}(\varepsilon_{\rm f}) d\varepsilon_{\rm f}$$



- Systematic survival probabilities have been calculated at optimal energies

C.J. Xia, B.X. Sun, E.G. Zhao, S.G. Zhou, Sci. Chin. Phys., 2011

- However, statistical model relies on parameterized level densities, fission barriers, temperature dependence…… and many corrections and associated parameters are introduced

- Microscopic Finite-Temperature Hartree-Fock-Bogoliubov can describe the thermal equilibrium compound nuclei: quantum effects (superfluidity and shell effects) can self-consistently and gradually disappear

A. L. Goodman, NPA 352, 30 (1981).

J. L. Egido, et al., PRL 85, 26 (2000).

$$\rho(\mathbf{r}) = \sum_i [f_i |U_i(\mathbf{r})|^2 + (1 - f_i)|V_i(\mathbf{r})|^2]$$

$$\tilde{\rho}(\mathbf{r}) = -\sum_i (1 - 2f_i) V_i(\mathbf{r}) U_i^*(\mathbf{r})$$

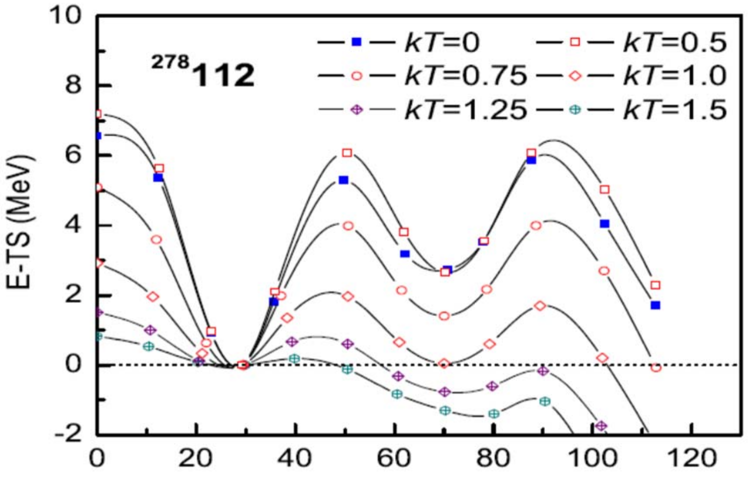
$$f_i = \frac{1}{1 + e^{(E_i/kT)}} \qquad S = -k \sum_i [f_i \ln f_i + (1 - f_i) \ln(1 - f_i)].$$

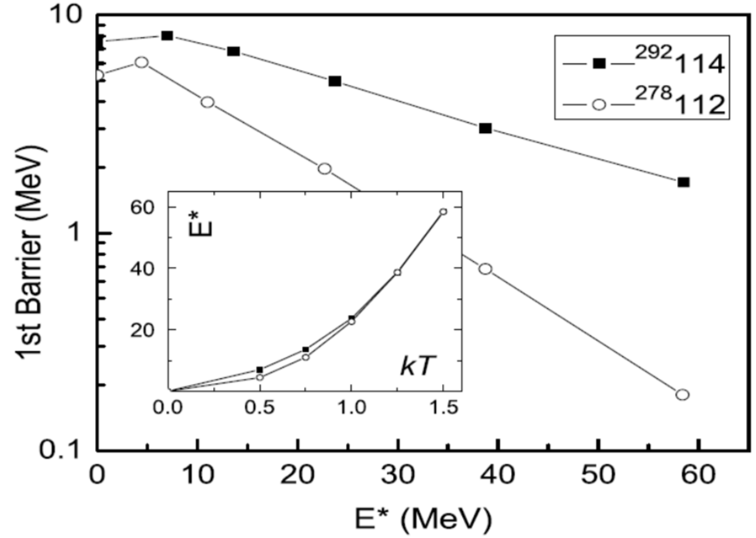
- Microscopic Finite-Temperature Skyrme Hartree-Fock-Bogoliubov can naturally describe the temperature dependent fission barriers and neutron gas at surfaces, without free parameters

$$F = E - TS$$ Fission barriers in terms of free energy

- **Microscopic thermal fission barriers**

J. C. Pei, W. Nazarewicz, J. A. Sheikh, and A. K. Kerman, PRL102, 192501 (2009).





- The temperature dependence of fission barrier heights are different for specific nuclei, due to quantum shell effects at high temperatures.
- Usually in experimental analysis, a damping factor is introduced

$$B_f = B_{LD} - \delta W e^{-\gamma_D E^*}$$

M.G. Itkis, Yu. Ts. Oganessian and V.I. Zagrebaev, Phys. Rev. C **65**, 044602(2002).

From classical statistical to quantum statistical decays

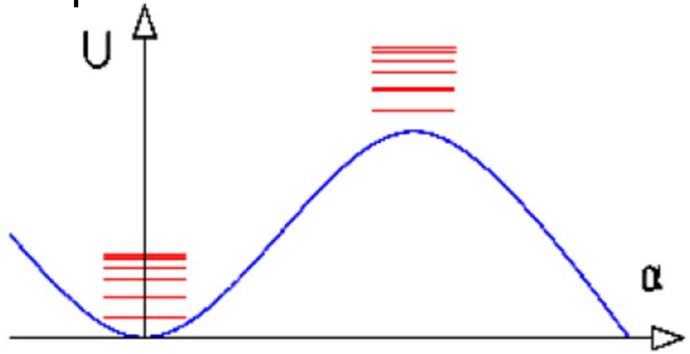
1. The Bohr-Wheeler transition state theory(1939)

fission barriers don't change with temperatures
depends on level densities at minimum and saddle points

Level density at saddle point is not know

$$\Gamma_f = \frac{1}{2\pi}\frac{1}{\rho_{CN}(E)}\int_0^{E-B_f}\rho_{sad}(E-B_F-\varepsilon)\,d\varepsilon$$

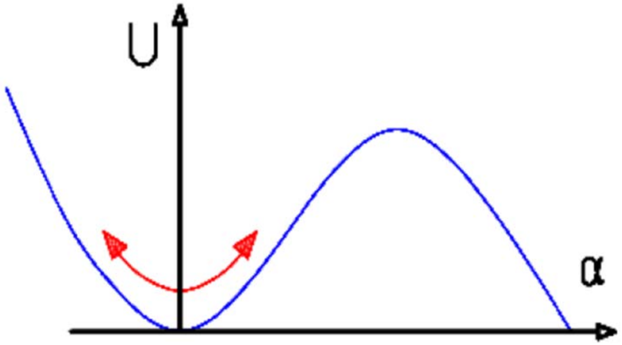
$$\Gamma_f = \frac{T}{2\pi}e^{-B_f/T}$$



2. The dynamic Kramers theory (related to Fokker-Planck)(1940)

consider the influences of barrier widths and dissipation
consistent or inconsistent with B-W without dissipation?

Strutinsky(1973)



$$\Gamma_K^{stat} = \frac{\hbar\omega_{gs}}{2\pi}e^{-B_f/T}$$

$$\Gamma_K = \Gamma_K^{stat}\cdot\left(\sqrt{1+\left(\frac{\beta}{2\omega_{sad}}\right)^2}-\frac{\beta}{2\omega_{sad}}\right)$$

3. The Imaginary Free Energy method (Im*F*)

A general theory at all temperatures for metastable systems(chemical reactions)

A more strict quantum treatment; fission barriers in free energy

Connected to Kramers theory at high temperatures

A transition temperature: from quantum tunneling to thermal decays

$$Z = \sum_n e^{-\beta z_n} = \sum_n e^{-\beta(E_n - i\hbar\gamma_n/2)} \qquad F = -(1/\beta)\ln Z$$

J.S. Langer, Ann. Phys. (N.Y.) 41, 108(1967).

I. Affleck, Phys. Rev. Lett 46, 388 (1981)

Our objective: microscopic study thermal fission rates (Im*F*) with the temperature dependent fission barriers and thermal neutron emission rates, and then survival probabilities, instead of conventional statistical models

Overview of Microscopic Fission studies

A well-known challenge for nuclear many-body theory towards a predictive microscopic fission theory

Review: N. Schunck, and L. M. Robledo, arXiv:1511.07517v2.

- Fission is a large amplitude collective motion
- Spontaneous fission has been extensively studied as a quantum tunneling process.
- Non-adiabatic studies: real-time dynamics only applicable after saddle points for fragment distributions (TD-HFB)
- Adiabatic DFT have to identify the neck and scission mechanism

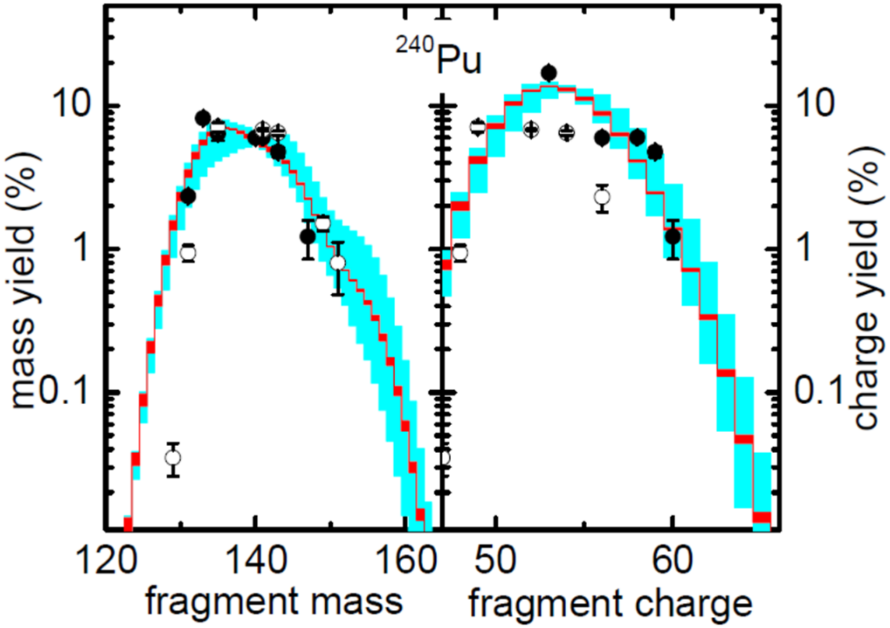
Two essential inputs:

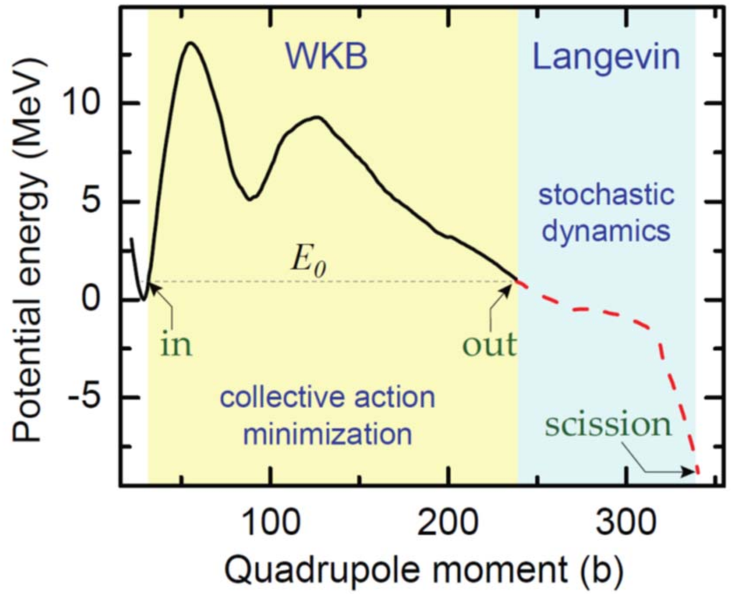
- Microscopic DFT studies of mass inertial parameters：cranking approximation, GCM, ATDHFB, local QRPA
- Microscopic DFT studies of fission barriers: large deformation properties(and beyond mean-field corrections); multi-dimensional potential energy surfaces(q_{20}, q_{22}, q_{30})

Overview of Microscopic Fission studies

WKB + Langevin dynamics

Spontaneous fission fragments



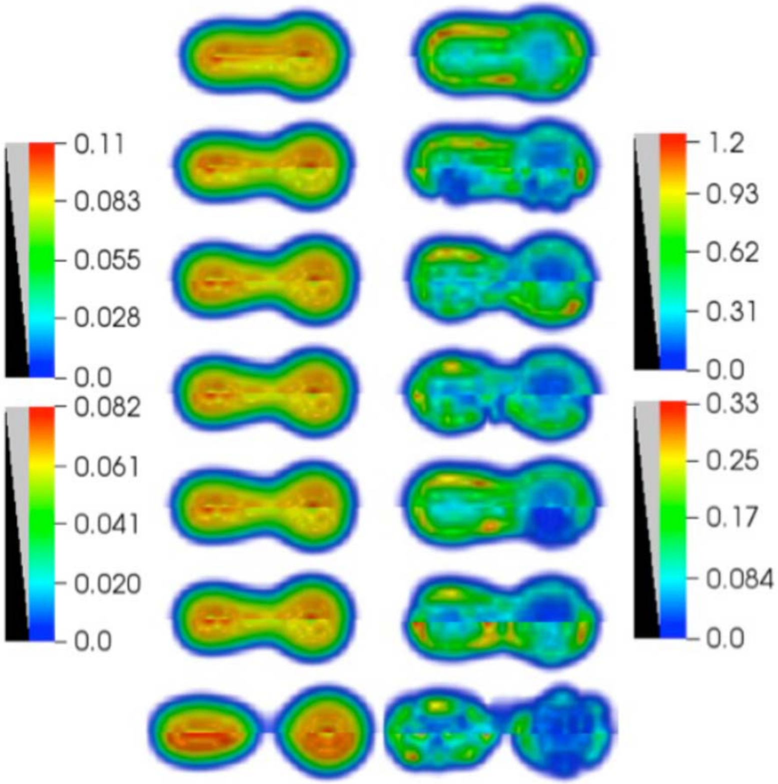


Jhilam Sadhukhan, Witold Nazarewicz, and Nicolas Schunck
Phys. Rev. C 93, 011304(R) (2016)

Overview of Microscopic Fission studies

TD-HFB

- Pairing is important: allow orbital changes （m,-m） - (m’, -m’)
- A large spherical fragment + a small deformed excited fragment
- Evolution time is longer than expected, not due to viscosity
- Nuclear forces are not sensitive



Aurel Bulgac, Piotr Magierski, Kenneth J. Roche, and Ionel Stetcu
Phys. Rev. Lett. 116, 122504 (2016)

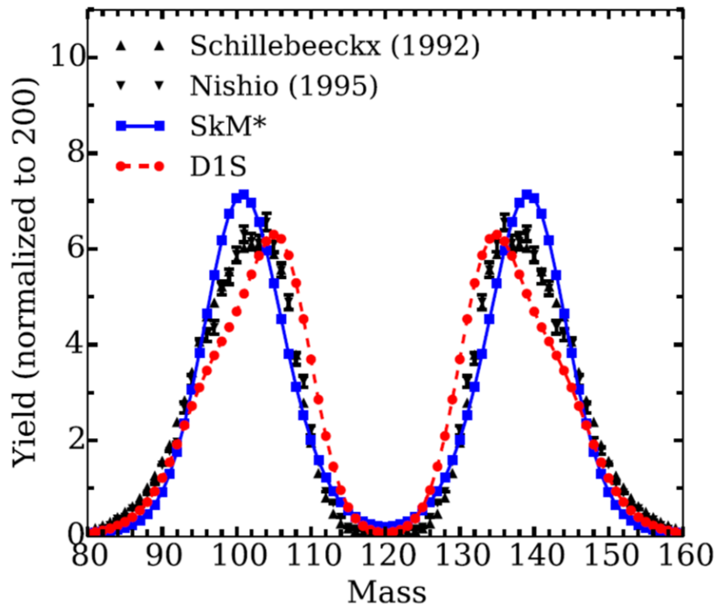
Overview of Microscopic Fission studies

TD-GCM

$$i\hbar\frac{\partial}{\partial t}g(\boldsymbol{q},t) = \left[-\frac{\hbar^2}{2}\sum_{\alpha\beta}\frac{\partial}{\partial q_\alpha}B_{\alpha\beta}(\boldsymbol{q})\frac{\partial}{\partial q_\beta} + V(\boldsymbol{q})\right] g(\boldsymbol{q},t).$$

$$F(\xi,t) = \int_{t=0}^{t} dT \int_{q\in\xi} \boldsymbol{J}(\boldsymbol{q},t)\cdot d\boldsymbol{S}.$$

- Adiabatic and no internal excitation
- Uncertainty of scission points
- Up to 2-dimensional and costly
- Suitable for fragment distribution

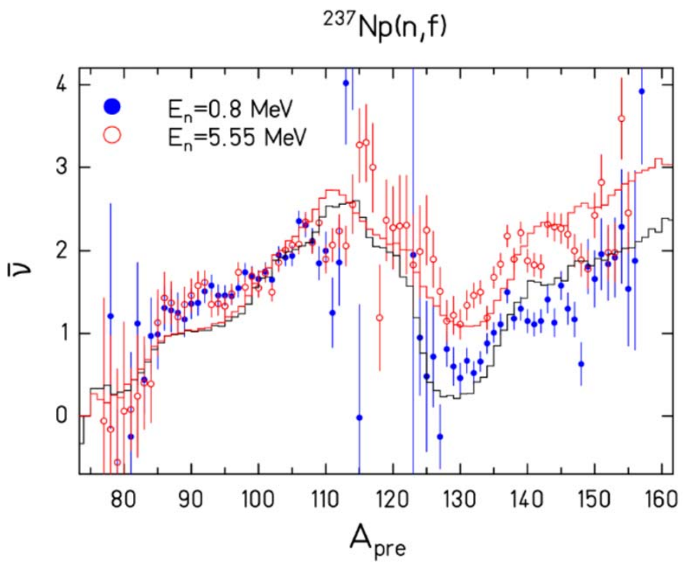


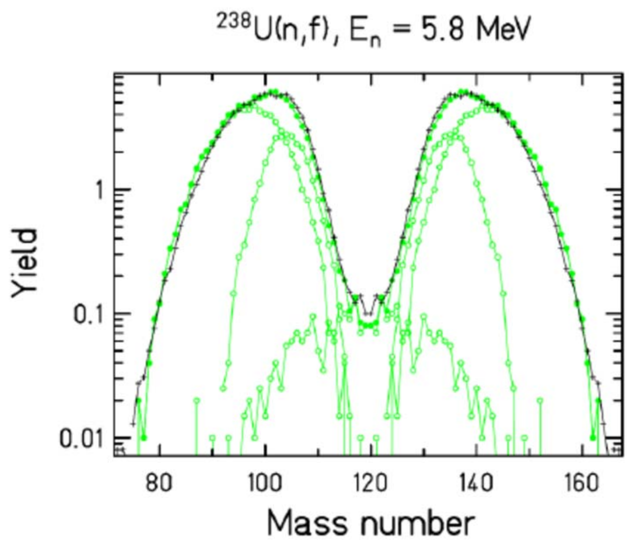
D. Regnier, N. Dubray, N. Schunck, and M. Verrière
Phys. Rev. C 93, 054611 (2016) -

Overview of Microscopic Fission studies

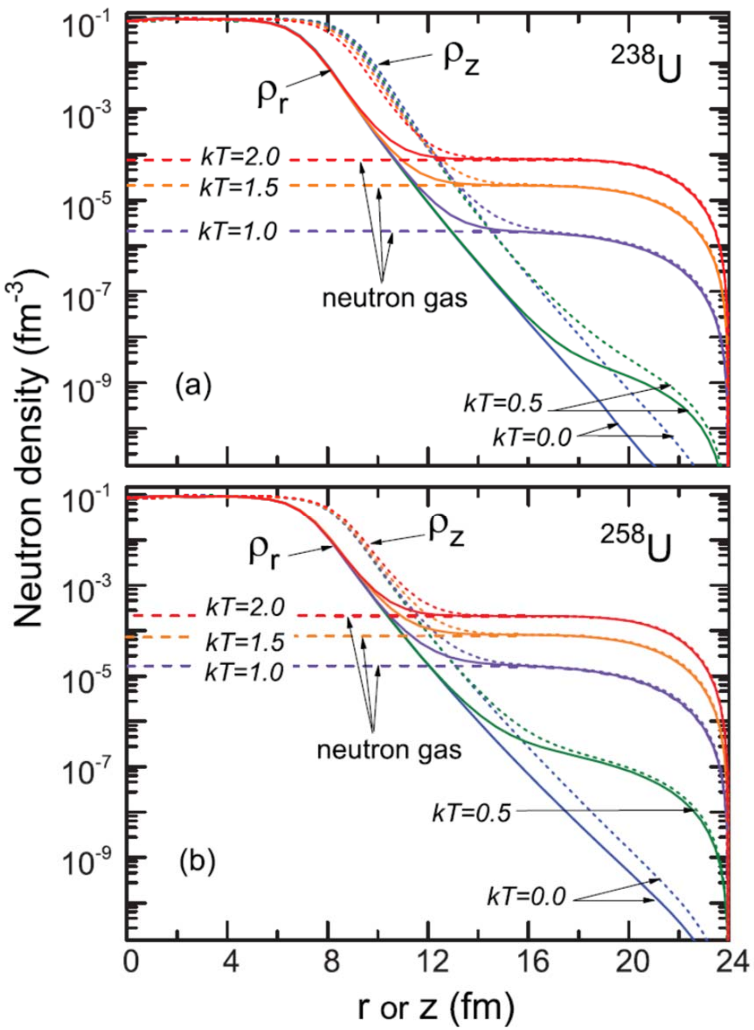
A number of libraries at the application level:
Level density; potential energy surface; shape before scission, Gaussian distribution, neck, potential curvature, dissipation …

Very wide applications:
Fission fragments, TKE, neutron emission, gammy emission…





Thermal neutron gas



- In FT-HFB, the thermal neutron gas at surfaces are generated to produce equilibrium pressure
- The neutron gases are unphysical, and should be subtracted from the system self-consistently
- The neutron emission (evaporation) rates is proportional to the gas density

Zhu, Pei, PRC, 90, 054316 (2014)

Thermal neutron emission rates

Statistical model:

$$\Gamma_n(E^*) = \frac{2mR^2}{\pi\hbar\rho(E^*)}\int_0^{E^*-B_n} \varepsilon\rho(E^* - B_n - \varepsilon)\mathrm{d}\varepsilon$$

$$\rho(E^*) = \frac{\sqrt{\pi}\exp(2\sqrt{aE^*})}{12a^{\frac{1}{4}}E^{*\frac{5}{4}}}$$

*J. L. Egido et al., J. Phys. G **19**, 1 (1993)*

Level density parameter:

$$a = \frac{A}{13}$$

S. Shlomo and J. B. Natowitz, Phys. Lett. B 252, 187 (1990)

FT-HFB approach:

$$\frac{\Gamma_n}{\hbar} = n_{gas} < \sigma v >$$

$$\langle v \rangle = \frac{\int f(\mathcal{E}_n)v(\mathcal{E}_n)\sqrt{\mathcal{E}_n}\,d\mathcal{E}_n}{\int f(\mathcal{E}_n)\sqrt{\mathcal{E}_n}\,d\mathcal{E}_n}$$

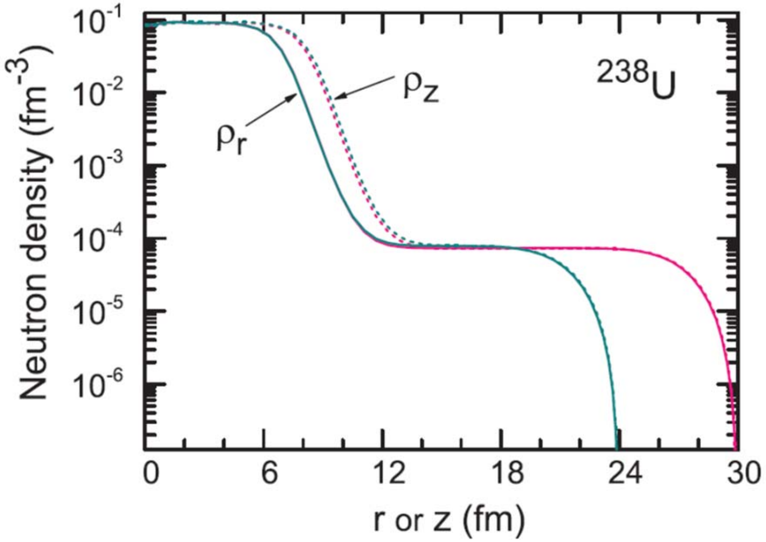
$$v(\mathcal{E}_n) = \sqrt{\frac{2\mathcal{E}_n}{m}}$$

$$f(\varepsilon_n) = \frac{1}{1+\exp(\frac{\varepsilon_n-\lambda_n}{kT})}$$

P.Bonche et al., NPA 427, 278 (1984)

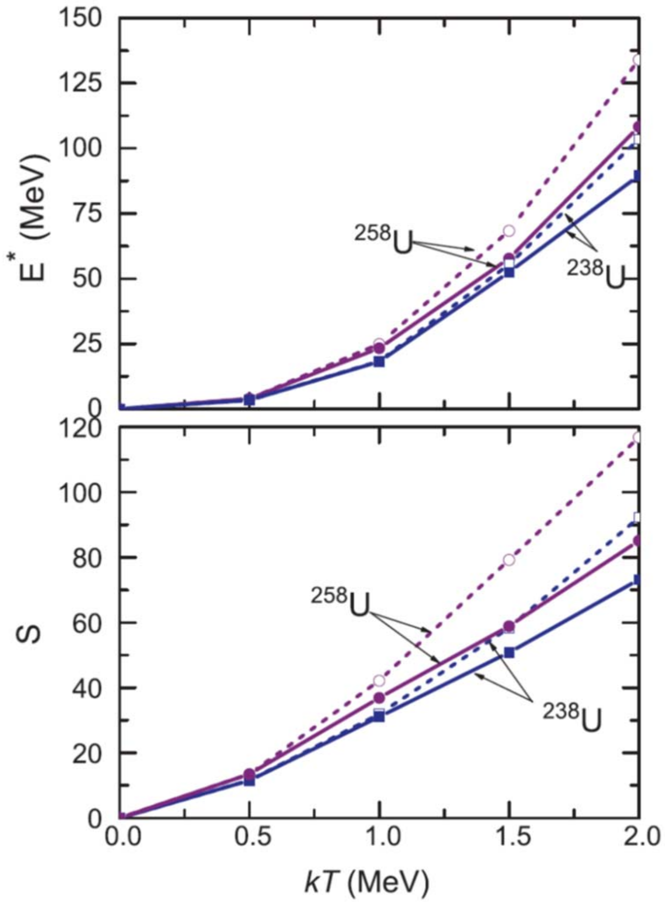
The level density parameter a, *which can be dependent on mass regions, deformations, and temperatures*

Treatment of neutron gas



$$Z = \int d^3r \left[\rho_p(\boldsymbol{r}) - \rho_p^{\mathrm{gas}}(\boldsymbol{r}) \right],$$

$$N = \int d^3r \left[\rho_n(\boldsymbol{r}) - \rho_n^{\mathrm{gas}}(\boldsymbol{r}) \right].$$



- A large box is required to get convergence for deformed cases.
- Self-consistent subtraction of gas is important for neutron-rich nuclei, large boxes and high temperatures.

Compare neutron emission rates

kT	FT-HFB		Stat-M	
(MeV)	n_{gas}	Γ	$\Gamma(a)$	$\Gamma(b)$
^{238}U				
1.0	2.07×10^{-6}	3.69×10^{-3}	1.11×10^{-3}	1.15×10^{-3}
1.5	2.09×10^{-5}	4.57×10^{-2}	6.15×10^{-2}	2.96×10^{-2}
2.0	7.67×10^{-5}	1.94×10^{-1}	2.56×10^{-1}	1.55×10^{-1}
^{258}U				
1.0	1.67×10^{-5}	3.16×10^{-2}	1.73×10^{-2}	1.02×10^{-2}
1.5	7.82×10^{-5}	1.82×10^{-1}	2.04×10^{-1}	1.10×10^{-1}
2.0	2.11×10^{-4}	5.70×10^{-1}	7.71×10^{-1}	4.10×10^{-1}

kT	FT-HFB		Stat-M	
(MeV)	n_{gas}	Γ	$\Gamma(a)$	$\Gamma(b)$
$^{278}_{112}$Cn				
1.0	5.53×10^{-7}	1.09×10^{-3}	1.36×10^{-4}	5.14×10^{-4}
1.5	8.84×10^{-6}	2.14×10^{-2}	2.76×10^{-2}	2.04×10^{-2}
2.0	3.76×10^{-5}	1.06×10^{-1}	2.21×10^{-1}	1.21×10^{-1}
$^{292}_{114}$Fl				
1.0	1.15×10^{-6}	3.69×10^{-3}	5.36×10^{-4}	9.04×10^{-4}
1.5	1.51×10^{-5}	3.79×10^{-2}	3.13×10^{-2}	2.64×10^{-2}
2.0	5.45×10^{-5}	1.58×10^{-1}	2.51×10^{-1}	1.48×10^{-1}

Zhu, Pei, PRC, 2014

Statistical model:
(a) use a level density a=A/13
(b) use a level density a=E/T^2
from FT-HFB calculations (*a connection*)

- Generally agree with the statistical results, however, with detailed differences…
- Microscopic results without any parameters.
- Level density parameters are difficult to be determined experimentally

Compare neutron emission rates

Statistical model and microscopic model:

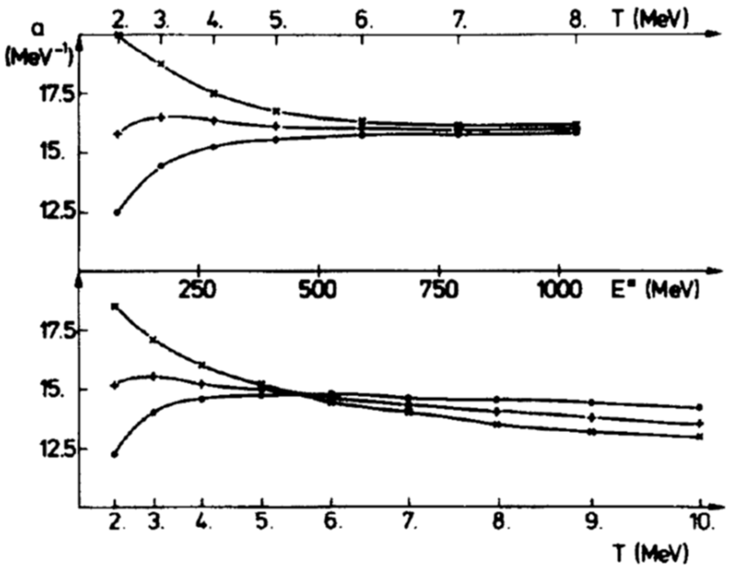
level density $a=E/T^2$ from FT-HFB calculations (*a connection*)

$$\rho(E^*) = \frac{\sqrt{\pi}\exp(2\sqrt{aE^*})}{12a^{1/4}E^{*5/4}}$$

large small

$$\boxed{a = \frac{S}{2T}, a = \frac{E^*}{T^2} \quad a = \frac{S^2}{4E^*}}$$

Microscopic
energy dependence



P. BONCHE et al, NPA , 1984

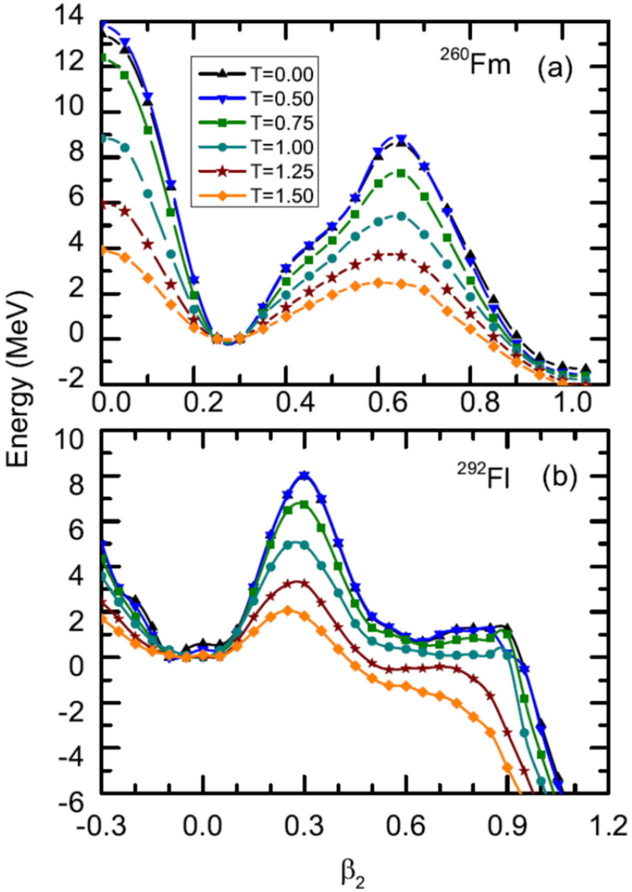
Thermal fission studies

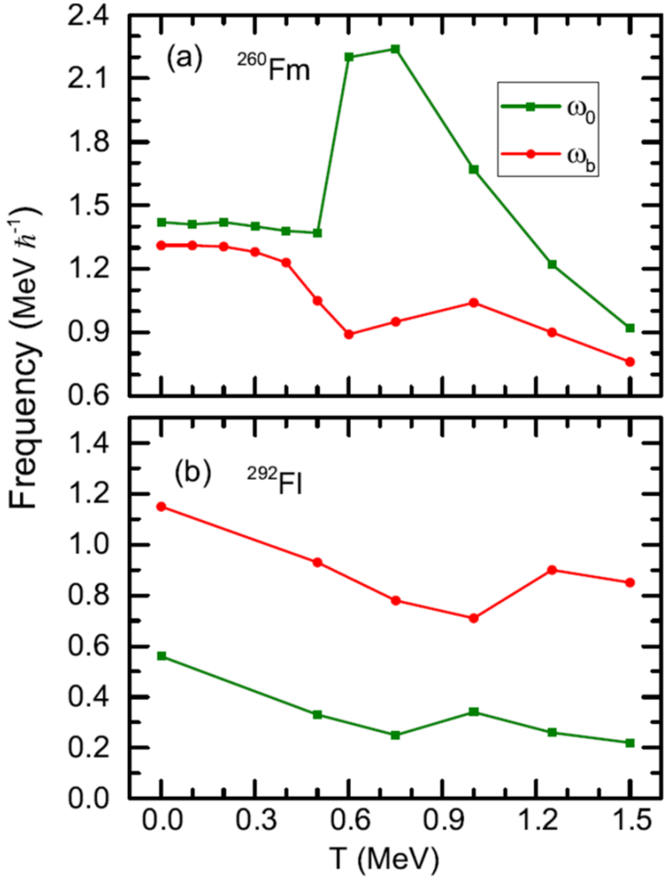
- Thermal fission involves all the issues of the spontaneous fission
- Gradually evolve from quantum tunneling to statistical escape mechanism
- Wide application interests: fast-neutron induced fission in reactors, fission in astrophysical environments, hot-fusion of superheavy nuclei
- Conventional studied by Bohr-Wheeler transition state theory and later the dynamical Kramers theory
- We use the imaginary free energy theory that is more microscopic and general for all temperatures.

I. Affleck, Phys. Rev. Lett 46, 388 (1981).

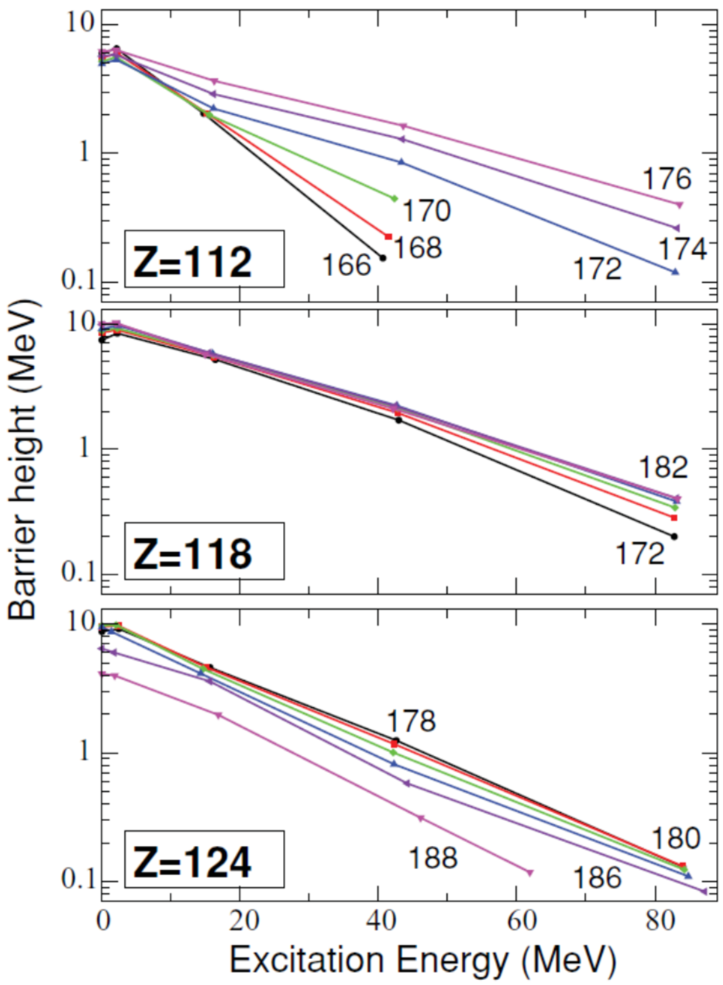
Microscopic Finite-Temperature Skyrme-HF+BCS studies of fission barriers

- Temperature dependent fission barrier heights, pathways (Pei, et al, PRL, 2009)
- Temperature dependent fission barrier curvatures (frequency) are also important inputs but has rarely been discussed. (Zhu, Pei, PRC, 2016)



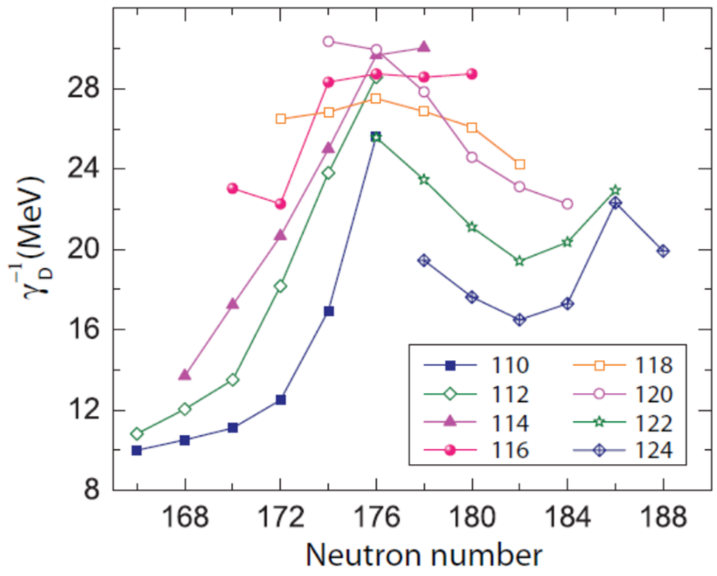


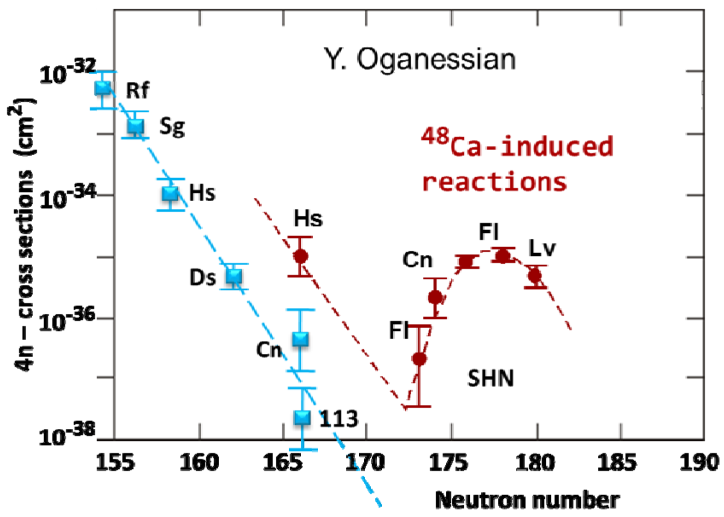
Systematic fission barriers



J. A. Sheikh, W. Nazarewicz, and J. C. Pei
Phys. Rev. C 80, 011302(R) (2009)

the surprise N=176





Mass parameters

Perturbative cranking approximations for mass parameters

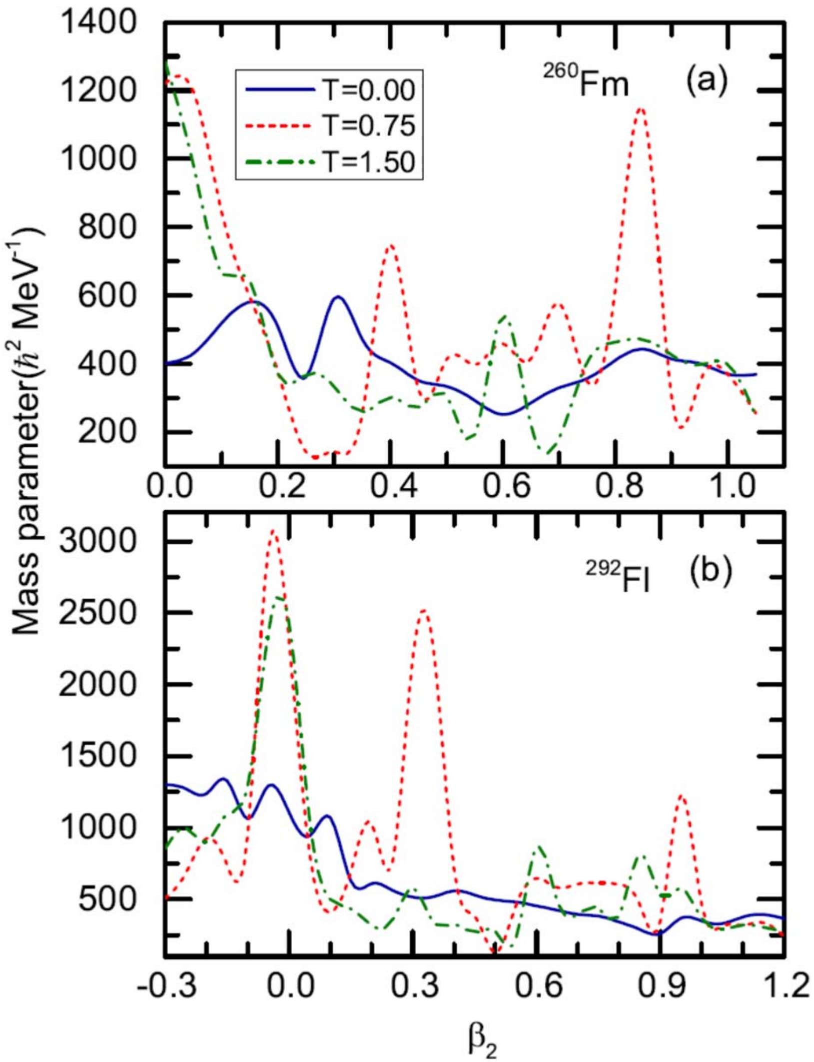
$$M_{20} = \hbar^2[\mathcal{M}^{(1)}]^{-1}[\mathcal{M}^{(3)}][\mathcal{M}^{(1)}]^{-1}$$

$$\mathcal{M}_{ij}^{(K)} = \frac{1}{2}\sum \frac{< 0|Q_i|\mu\nu >< \mu\nu|Q_j|0 >}{(E_\mu + E_\nu)^K}(u_\mu v_\nu + u_\nu v_\mu)^2$$

Finite-Temperature cranking approximations for mass parameters

$$\begin{aligned}\mathcal{M}_{ij,T}^{(K)} &= \frac{1}{2}\sum < 0|Q_i|\mu\nu >< \mu\nu|Q_j|0 > \\ &\left\{\frac{(u_\mu u_\nu - v_\mu v_\nu)^2}{(E_\mu - E_\nu)^K}[\tanh(\frac{E_\mu}{2kT}) - \tanh(\frac{E_\nu}{2kT})]\right. \\ &\left. +\frac{(u_\mu v_\nu + u_\nu v_\mu)^2}{(E_\mu + E_\nu)^K}[\tanh(\frac{E_\mu}{2kT}) + \tanh(\frac{E_\nu}{2kT})]\right\}\end{aligned}$$

Mass parameters



- As the pairing disappears, the mass parameters increase and become much irregular
- As the shell effects disappear, the mass parameters decrease and become like irrotational liquid

Thermal fission rates at all temperatures

Imaginary Free energy (ImF) decays

$$\boxed{\Gamma = [2\sinh(\frac{1}{2}\beta\hbar\omega_0)]\frac{1}{2\pi\hbar}\int_0^{V_b} P(E)\exp(-\beta E))dE}$$

The ImF formula at high temperatures

$$\boxed{\Gamma = \frac{\omega_b}{2\pi}\frac{\sinh(\frac{1}{2}\beta\omega_0)}{\sin(\frac{1}{2}\beta\hbar\omega_b)}\exp(-\beta V_b)}$$

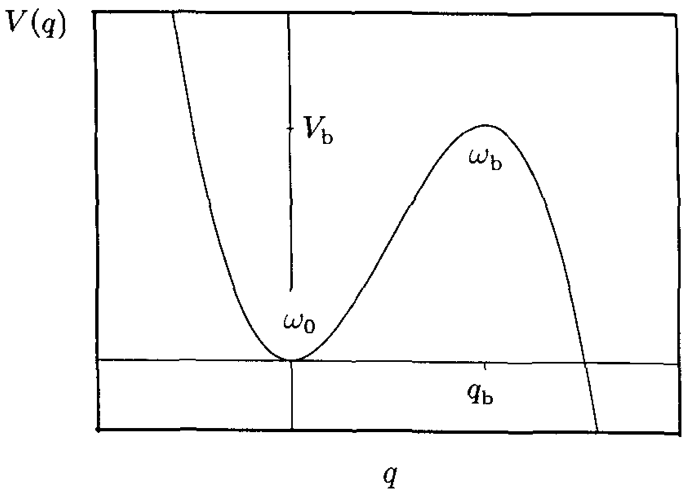
The Kramers formula

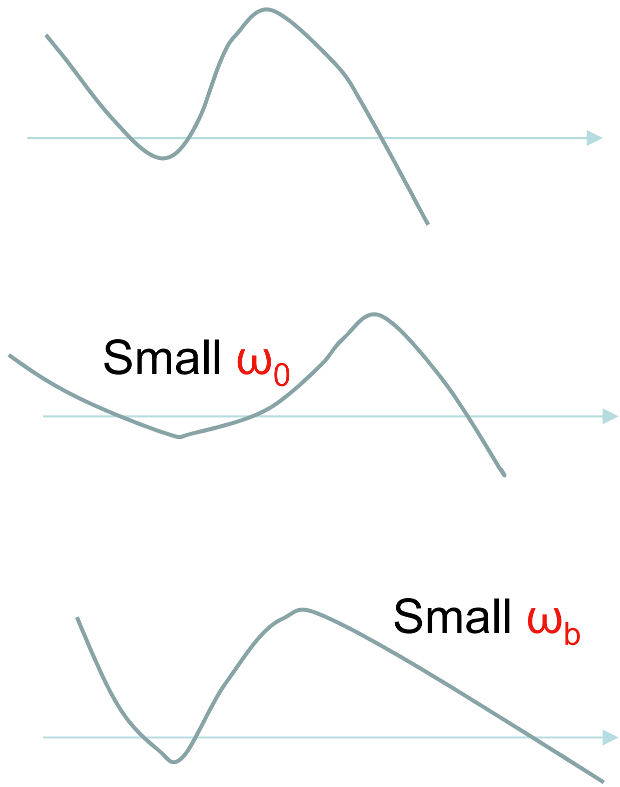
$$\Gamma_{\mathrm{Kramers}} = \frac{\omega_0}{2\pi}\exp(-\beta V_b)$$

I. Affleck, Phys. Rev. Lett 46, 388 (1981).

Temperature dependent potential curvatures

Curvatures are important!





- Barrier reflection can be considered by a parabolic potential
- The ω_b has not been considered in Bohr-Wheeler formula

- Curvatures are now obtained microscopically
- Both ω_0, ω_b are decreasing and play a role as dissipation

Microscopic fission lifetimes

T	^{260}Fm		^{240}Pu	
(MeV)	E*	T_f(s)	E*	T_f(s)
0.1	0.001	1.50×10^{-3}	0.002	2.55×10^{10}
0.2	0.11	1.59×10^{-6}	0.13	2.80×10^{-3}
0.3	0.83	3.67×10^{-10}	0.81	4.50×10^{-8}
0.4	2.67	1.94×10^{-12}	2.43	3.48×10^{-10}
0.5	5.67	7.87×10^{-14}	4.85	9.08×10^{-11}
0.6	8.63	3.48×10^{-15}	7.02	8.17×10^{-12}
0.75	10.91	2.07×10^{-16}	11.19	9.61×10^{-13}

- Nuclei with different curvatures can have different critical temperatures:

$$T_c = \omega_b/2\pi$$

- For Pu240, with a very low critical temperature and lifetime deceases very rapidly. Low temperature ImF formula is not suitable.

Microscopic fission lifetimes

T	^{260}Fm		^{240}Pu	
(MeV)	E*	T_f(s)	E*	T_f(s)
0.3	0.83	1.90×10^{-9}	0.81	3.25×10^{-8}
0.4	2.67	4.90×10^{-12}	2.43	2.92×10^{-11}
0.5	5.67	9.03×10^{-14}	4.85	4.51×10^{-13}
0.6	8.63	1.85×10^{-15}	7.02	5.51×10^{-15}
0.75	10.91	1.11×10^{-17}	11.19	8.13×10^{-17}
1.0	23.92	4.72×10^{-19}	21.22	1.12×10^{-18}
1.25	38.38	6.01×10^{-20}	35.42	9.14×10^{-20}
1.5	58.80	2.29×10^{-20}	54.40	3.27×10^{-20}
T	^{278}Cn		^{292}Fl	
(MeV)	E*	T_f(s)	E*	T_f(s)
0.5	4.70	3.54×10^{-17}	5.82	1.01×10^{-13}
0.75	11.25	3.56×10^{-19}	14.1	1.25×10^{-16}
1.0	23.17	2.32×10^{-20}	24.27	1.66×10^{-18}
1.25	40.17		40.22	2.09×10^{-19}
1.5	62.34		69.01	7.33×10^{-20}

4% (beside the ^{278}Cn row T = 1.0)

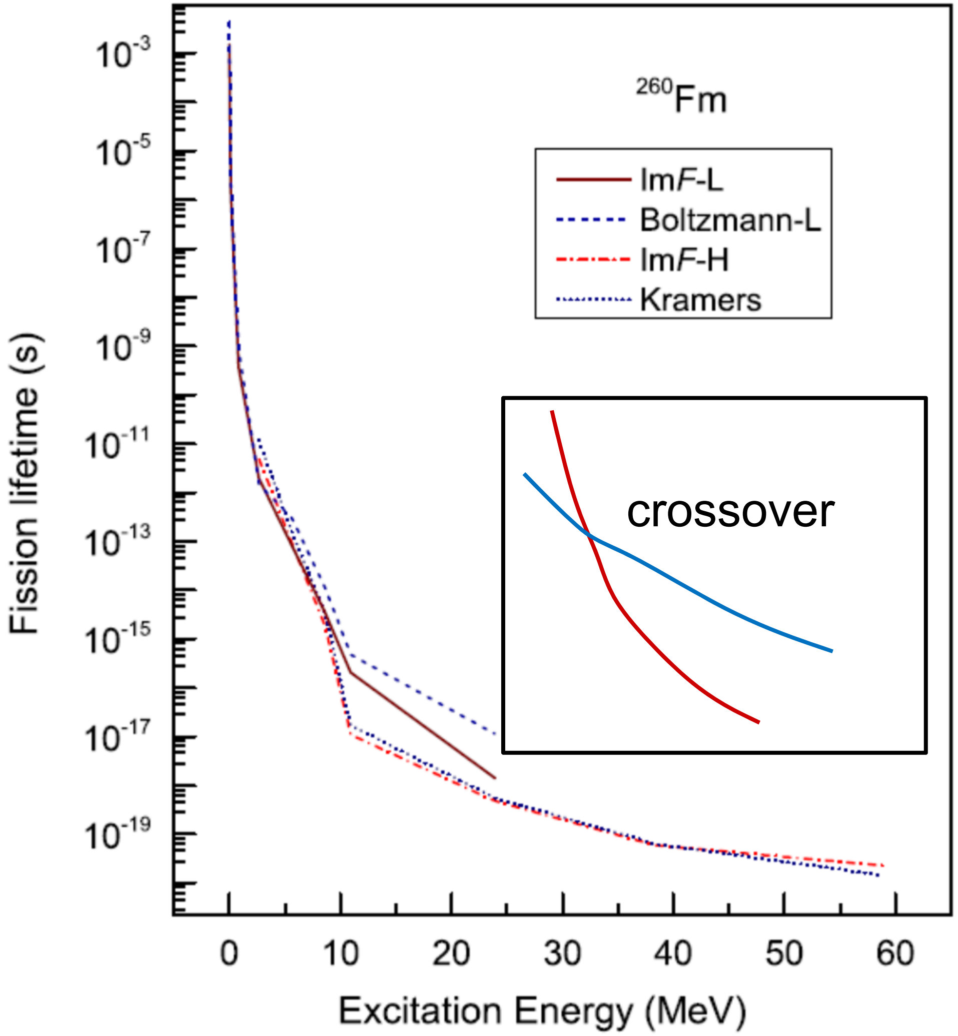
90% (beside the ^{292}Fl row T = 1.0)

81% (beside the ^{292}Fl row T = 1.5)

- Large difference in low temperatures; Small differences in high temperatures
- Quantum effects are important at low temperatures

- Large survival probabilities are obtained for 292Fl

Thermal fission: a transition



Zhu, Pei, PRC, 2016

- Fission lifetimes decrease very rapidly at low excitation energies
- A smooth connection between low-T formula and high-T formula.
- The applicability of low-T formula is slightly higher than T_c
- Kramers formula overestimate fission lifetime at low temperatures

^{274}Hs

Experiment Survival probability

Large experimental survival probability of 274Hs has been given at 63 MeV, R.Yanez, et al., PRL 112, 152702 (2014)

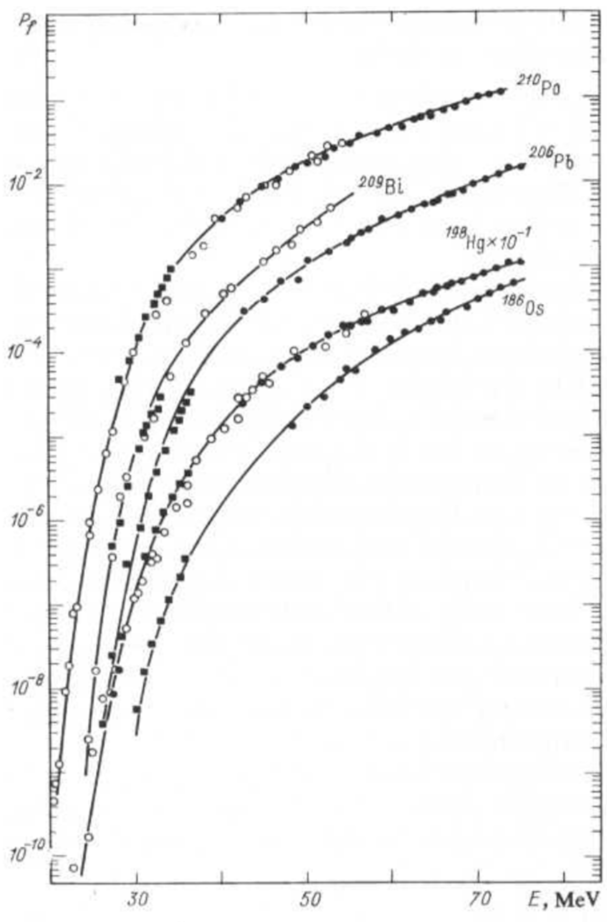
Statistical model: **23%**
Experiments: **89%**, large dissipation?

Identify the prescission and postscission components of the neutron multiplicities in each system Mg26+Cm248

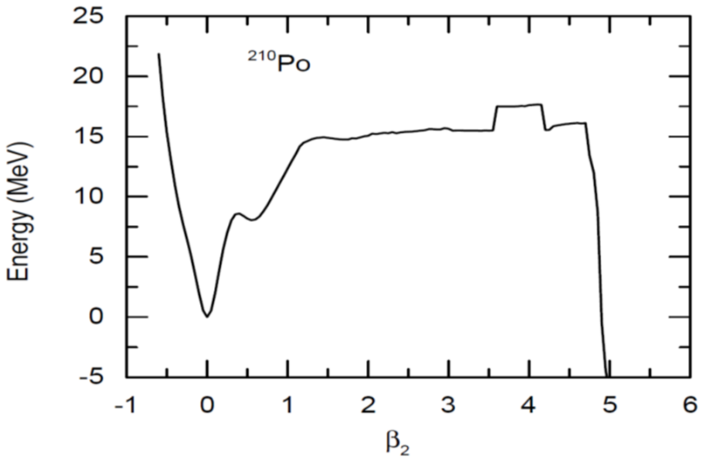
Our calculations: ~30%

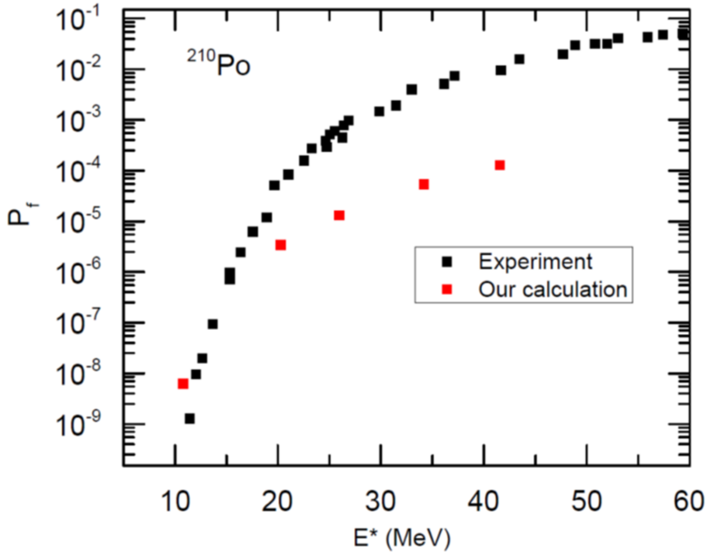
Many questions about this experimental data

^{210}Po



Sov. J. Part. Nucl. 16 (4), July–Aug. 1985

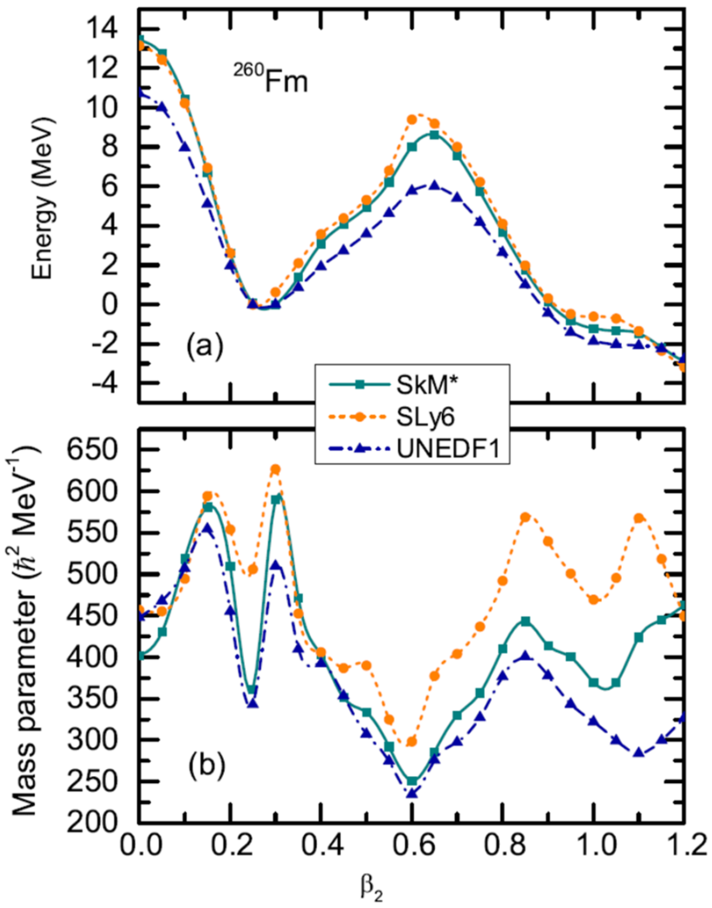




No free parameter; may have asymmetry fission
No angular momentum dependence yet

Uncertainties and open questions

Significant model dependences at spontaneous fission



What has been missed

- Full multi-dimensional
- ZPE corrections to barriers
- Time-odd effects to mass
- Non-adiabatic fission

Summary

- A roadmap towards microscopic descriptions of induced fission rates, based on temperature dependent fission barrier heights and curvatures, and mass parameters.
- Neutron emission rates in deformed nuclei is obtained, agree with statistical model
- Now we can derive the microscopic survival probability of compound superheavy nuclei without free parameters for the first time.

Outlook:

- Thermal fission in multi-dimensional deformation spaces,
- Fission lifetime and fragment distributions together
- We have dropped out the viscosity and dissipation which can be important at high temperatures.

Collaborations:

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Y. Zhu, Y.N. Zhang, X.Y. Xiong, K. Wang, N. Fei…..

And many others for discussions

Thank you for your attention !