西南大學

Study of Nuclear Fission Dynamics Within Relativistic Density Functional Theory

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2024.12

Where is Chongqing

Beautiful modern city




Delicious food…

Hot spring…

Contents

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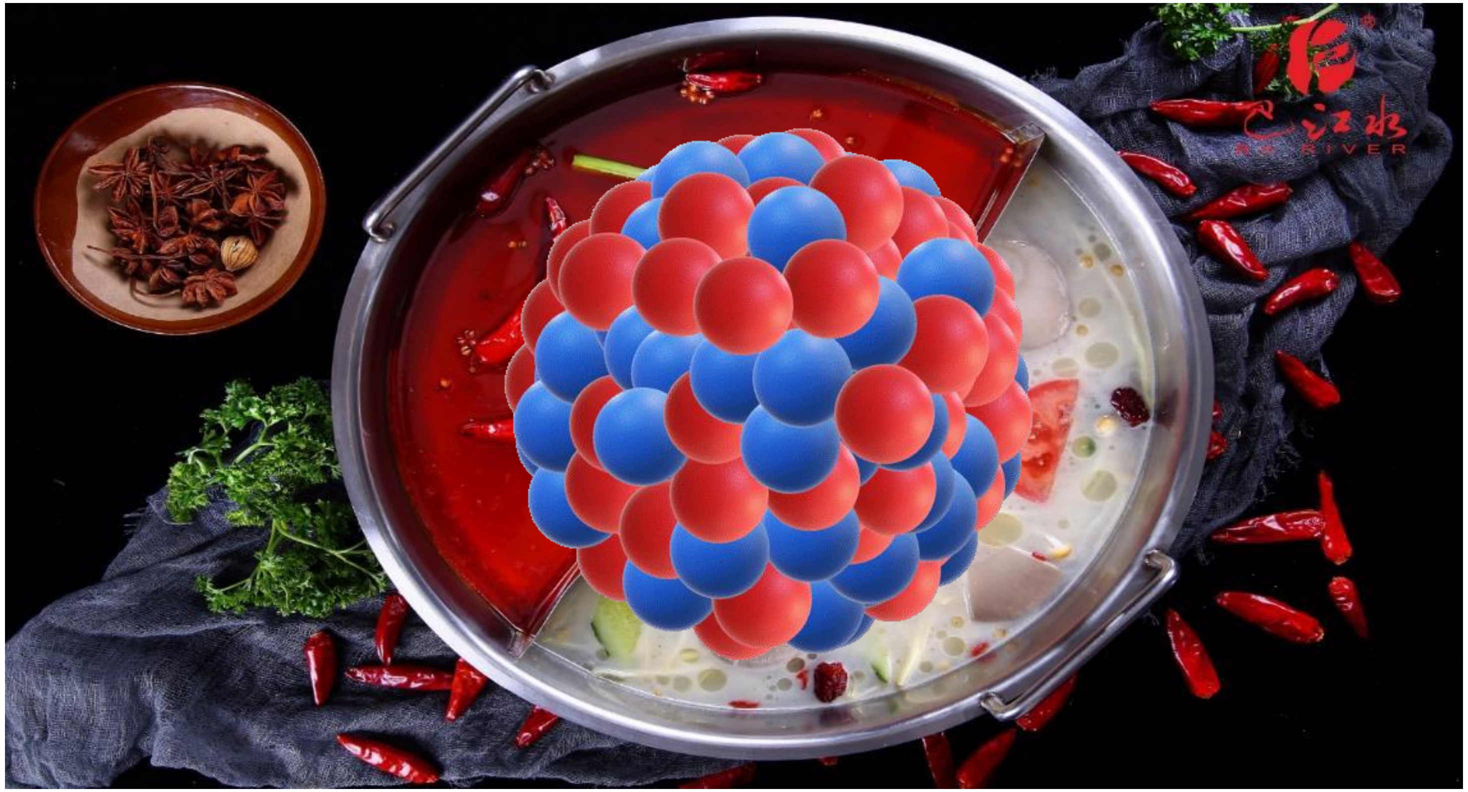
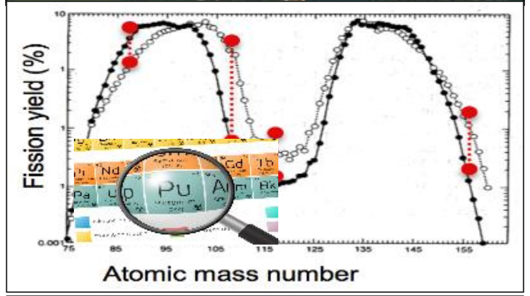
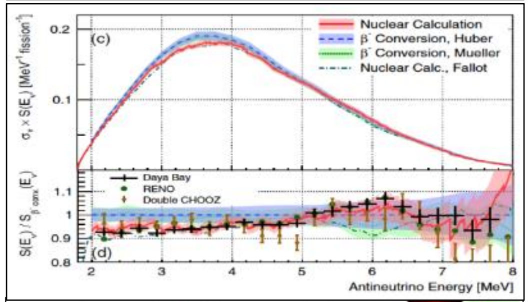


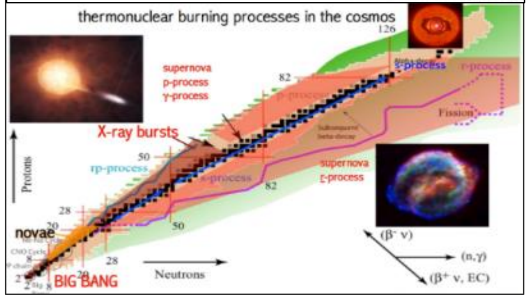
Contents

Application of Nuclear Fission

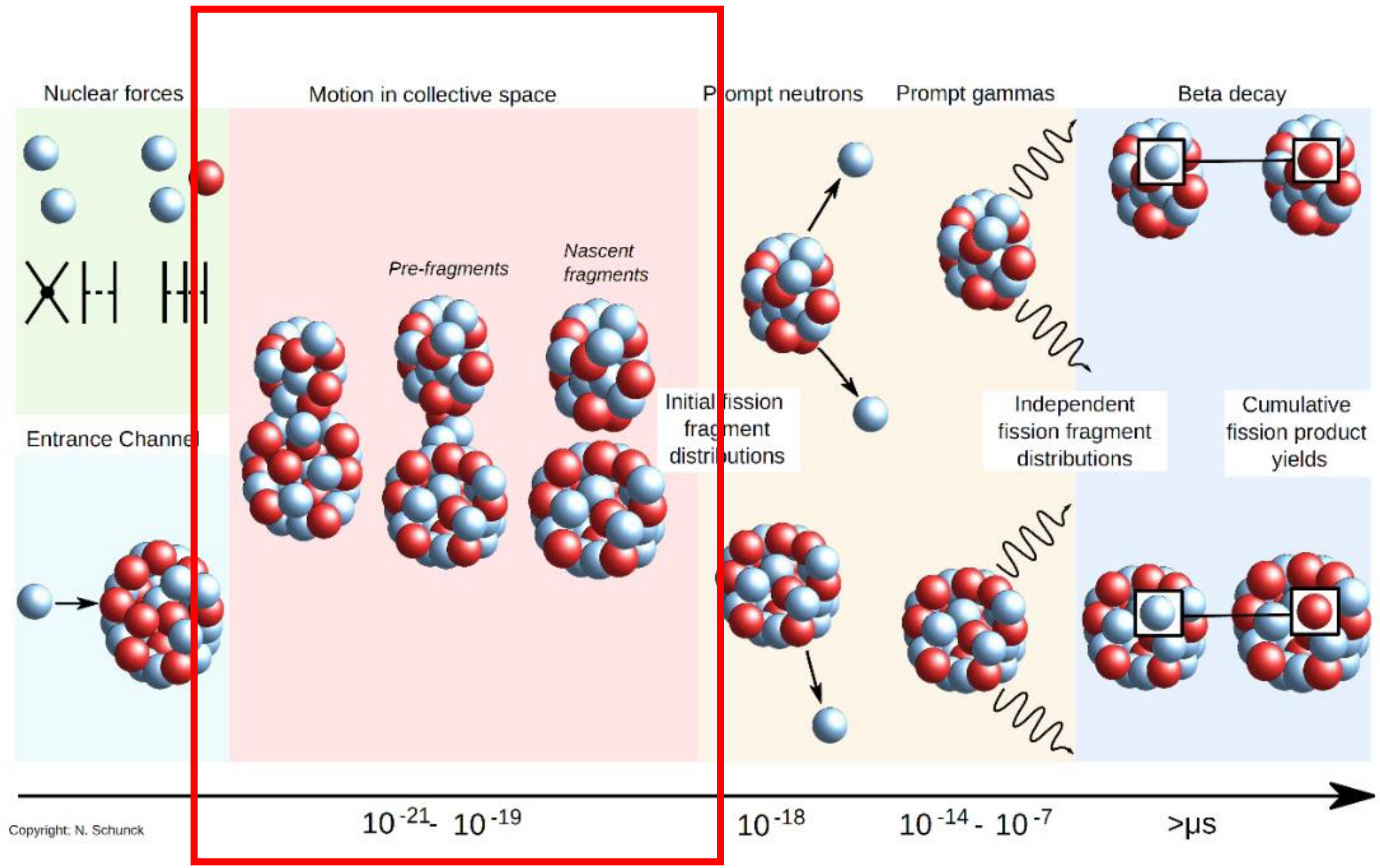
- **Reactor design and operation**
  - reactivity calculations, fuel and reactor core management, reactor safety (IND and CUM)
- **Reprocessing of spent fuel and nuclear waste management**
  - Fission product inventory, decay heat calculation (IND)
- **Safeguard**
  - monitor fission products for the verification (CUM)
- **Fundamental physics**
  - understanding fission physics, r-process nucleosynthesis, antineutrino anomaly (FY)， fission angular momentum …







Overview of the Nuclear fission process

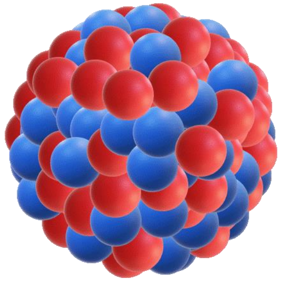


Neutron-induced fission process

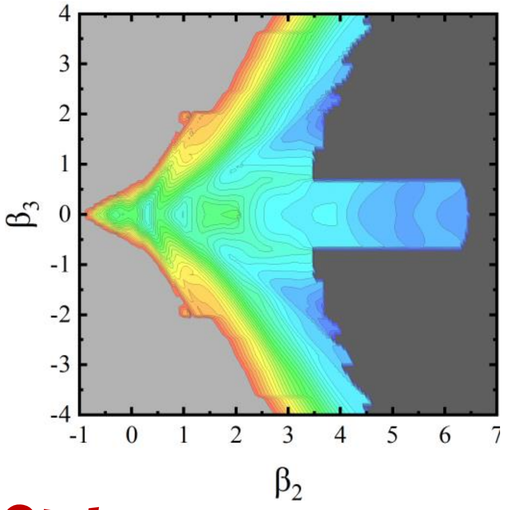
M. Bender et al., J. Phys. G 47, 113002 (2020)

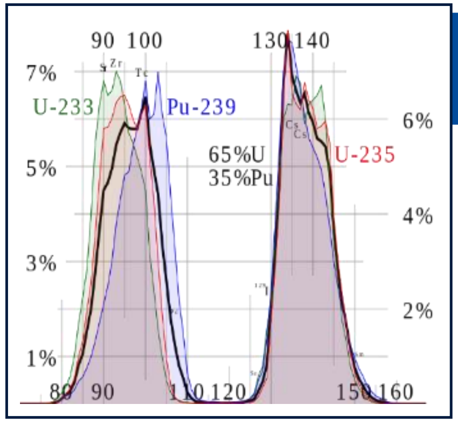
- **Nuclear fission: an atomic nucleus splits into two or more fragments.**
- **The process involves complex correlation, fluctuation, dissipation ...**

Frontiers of fission

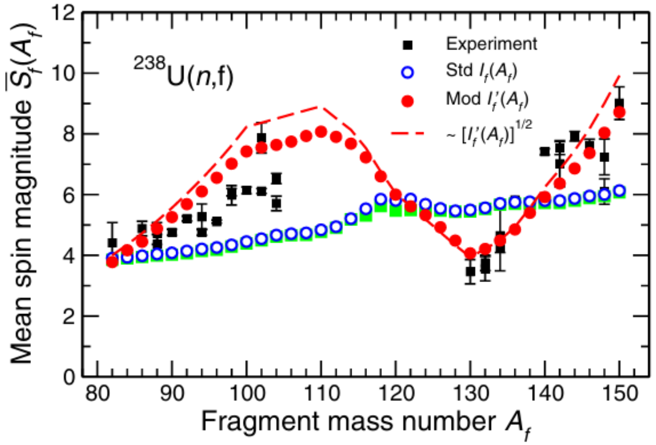


Dynamics

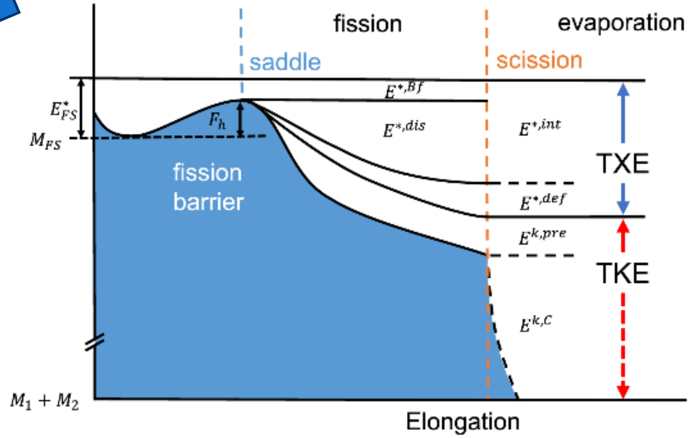




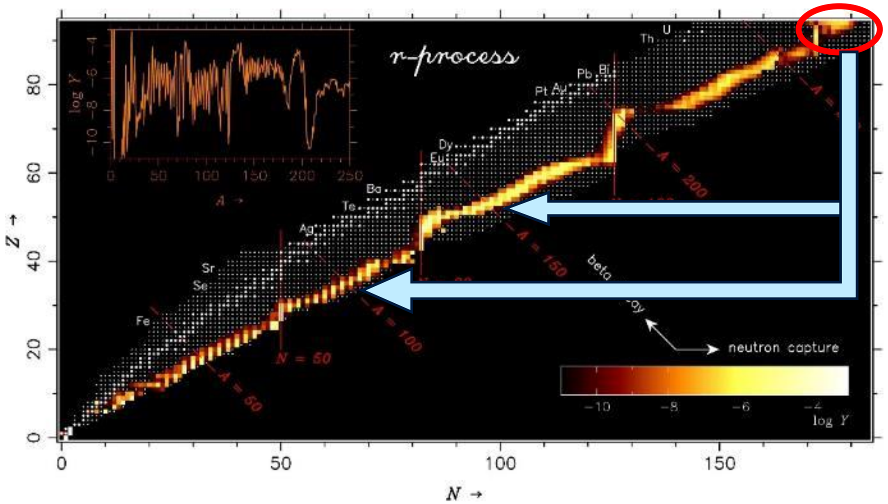
Angular momentum



Dissipation

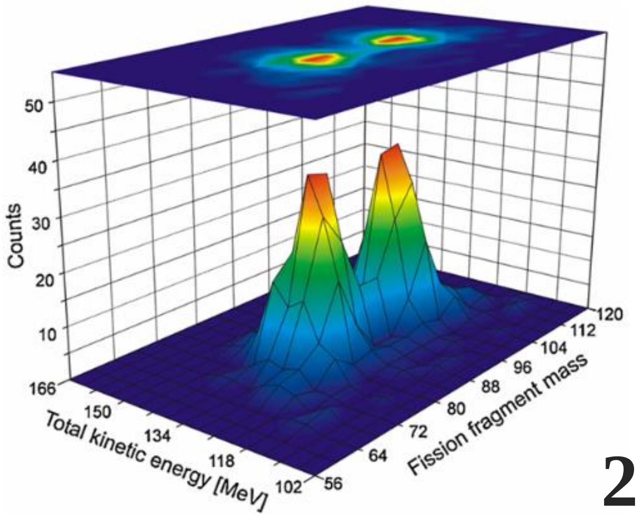


Intersection
with astrophysics



Progress in fission: Experiments & Observations

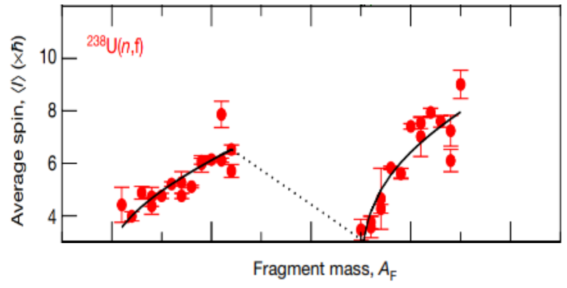
A. N. Andreyev *et al.* PRL 105, 252502(2010)



2010

New type asymmetric fission in the sub-lead region

J. N. Wilson, *et al.*, Nature 590, 566 (2021)



2021

Fragments' angular momenta

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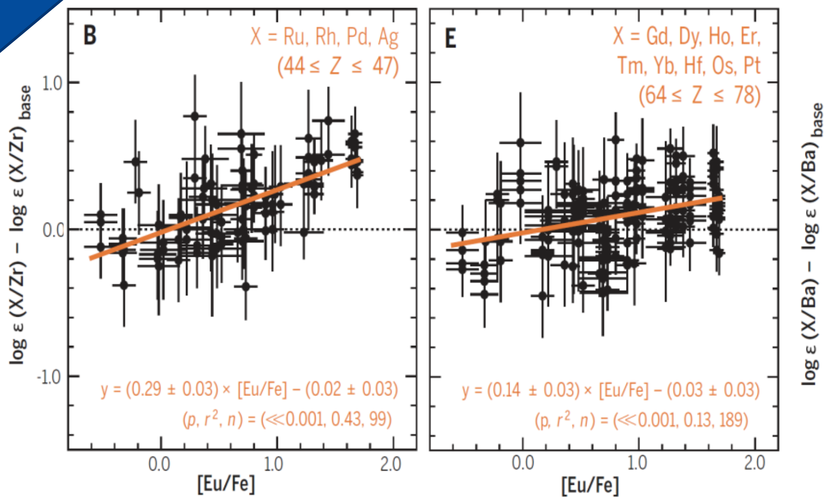
2023

Roederer *et al.*, Science 382, 1177–1180(2023)



Fission of transuranic nuclei is involved in the r process

Progress in fission: Theoretical Models

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➢ Statistical model

Viñas, B. M., & Caamaño, M. EPJA, 60(12), 237.(2024).
J. Randrup, T. Døssing, R. Vogt, PRC106, 014609(2022).
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H. Paşca, A. V. Andreev, G. G. Adamian, et al., PRC104, 014604(2021).
A. Dey, D. C. Biswas, A. Chakraborty, et al. PRC103, 044322 (2021).
J.F. Lemaître, S. Goriely, S. Hilaire et al., PRC99, 034612 (2019).
Y.W. Hao G.X. Dong, X.B. Wang, et al., SSPMA49, 122001(2019). ……

➢ Macro-micro model

Ivanyuk, F. A., and N. Carjan. arxiv:2411.04505 (2024).
X. Guan, T.C. Wang, W.Q. Jiang, et al. PRC107, 034307(2023).
K. Pomorski, B. Nerlo-Pomorska, C. Schmitt, et al. PRC107, 054616(2023).
Y. Aritomo, A. Iwamoto, K. Nishio, and M. Ohta, PRC105, 034604(2022).
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L.L. Liu, X.Z. Wu, Y.J. Chen, et al. PRC105, 034614(2022).
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M. Albertsson, B. G. Carlsson, T. Døssing, et al., PRC103, 014609(2021).
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C. Karthikraj, Z.Z. Ren, et al. PRC101, 014603(2020).
K. Pomorski, A. Dobrowolski, R. Han, et al., PRC101, 064602(2020).
M. R. Mumpower, P. Jaffke, M. Verriere, et al., PRC101, 054607(2020) .
C. Ishizuka, X. Zhang, M.D. Usang, et al., PRC101, 011601(R)(2020).
Z.M. Wang, W.J. Zhu, C.L. Zhong, et al. NPA989, 81-96(2019). ……

➢ Microscopic model (DFT)

Ibrahim, Matthew and Bulgac, et al.,PRL132,242501(2024).
Godbey, K, A. S. Umar,et al. PRC110,L041601(2024).
B. Li, D. Vretenar, T. Nikšić, et al. FP19, 44201 (2024).
X. B. Wang, Y.J. Chen, G. X. Dong, et al. PRC108, 034306(2023).
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Y. Iwata, T. Nishikawa, PRC105, 044603(2022).
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A. Bulgac, I. Abdurrahman, K. Godbey, et al. PRL128, 022501(2022).
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Y. Qiang, J. C. Pei, P. D. Stevenson, PRC103, L031304(2021).
F. Mercier, J. Zhao, J. P. Ebran, et al., PRL127, 012501 (2021).
A. Bulgac, I. Abdurrahman, S. Jin, et al., PRL126, 142502(2021).
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➢ Machine learning

Tsioulos, V., and V. Prassa. EPJ Web Conf. 304, 01015 (2024)
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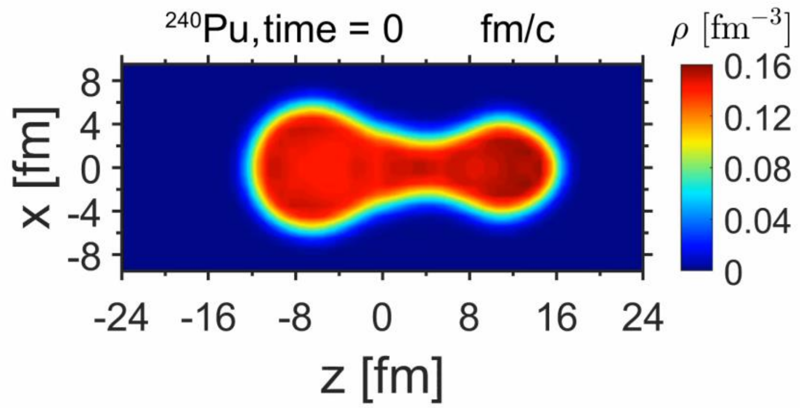
Microscopic models for fission dynamics

➢ Time-Dependent Density Functional Theory (TDDFT)

Time evolution of intrinsic spatial wave functions (densities)



J. W. Negele, S. E. Koonin, P. Möller, *et al*., PRC17, 1098 (1978).
A.Bulgac, P. Magierski, K. J. Roche *et al*., PRL116, 122504 (2016)
T. Nakatsukasa, K. Matsuyanagi,*et al*, RMP. 88, 045004 (2016)
G. Scamps, C. Simenel, Nature 564,382(2018).
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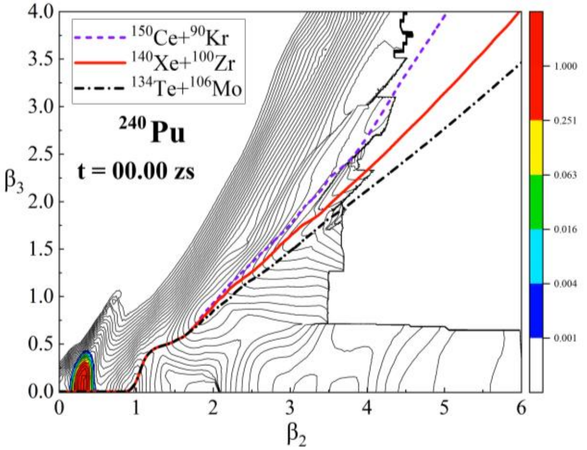
Y. Huang, X. X. Sun, L. Guo, EPJA60, 100(2024) ……

➢ Time-Dependent Generator Coordinate Method (TDGCM)

Time evolution of the probability wave packet in collective space.



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H. Goutte, J. F. Berger, P. Casoli, et al., PRC71,024316 (2005)
H. Tao, J. Zhao, Z. P. Li, *et al*., PRC96,024319 (2017)
A.Zdeb, A. Dobrowolski, M. Warda, PRC95,054608 (2017)
J. Zhao, T. Nikšić, D. Vretenar, S.G. Zhou, PRC101, 064605(2020)
Y.J. Chen , Y. Su , L.L. Liu, et al., CPC47 054103(2023)
X. B. Wang, Yongjing Chen, G. X. Dong, PRC108, 034306(2023)
B. Li, D. Vretenar, T. Nikšić, et. al., FP19, 44201(2024)
Bulgac, Aurel.arxiv preprint arxiv:2408.02173 (2024) ……

Contents

Relativistic Density Functional Theory (RDFT)

- **Relativistic energy density functional**

$$
\begin{aligned}
E_{\mathrm{CDF}} &= \int d\mathbf{r}\,\varepsilon_{\mathrm{CDF}}(\mathbf{r}) \\
&= \sum_k \int d\mathbf{r}\, v_k^2 \bar{\psi}_k(\mathbf{r})(-i\gamma\nabla + m)\psi_k(\mathbf{r}) \\
&+ \int d\mathbf{r} \left(\frac{\alpha_S}{2}\rho_S^2 + \frac{\beta_S}{3}\rho_S^3 + \frac{\gamma_S}{4}\rho_S^4 + \frac{\delta_S}{2}\rho_S\Delta\rho_S \right. \\
&+ \frac{\alpha_V}{2} j_\mu j^\mu + \frac{\gamma_V}{4}(j_\mu j^\mu)^2 + \frac{\delta_V}{2} j_\mu \Delta j^\mu + \frac{e}{2}\rho_p A^0 \\
&\left. + \frac{\alpha_{TV}}{2} \vec{j}^{\mu}_{TV}\cdot(\vec{j}_{TV})_\mu + \frac{\delta_{TV}}{2}\vec{j}^{\mu}_{TV}\cdot\Delta(\vec{j}_{TV})_\mu \right)
\end{aligned}
$$

ρ_S, j^μ, $\vec{j}^{\mu}_{TV}$: **Density and currents of nucleons**

$\alpha, \beta, \gamma, \delta$: **Coupling constants (PC-PK1, DD-PC1, etc.)**

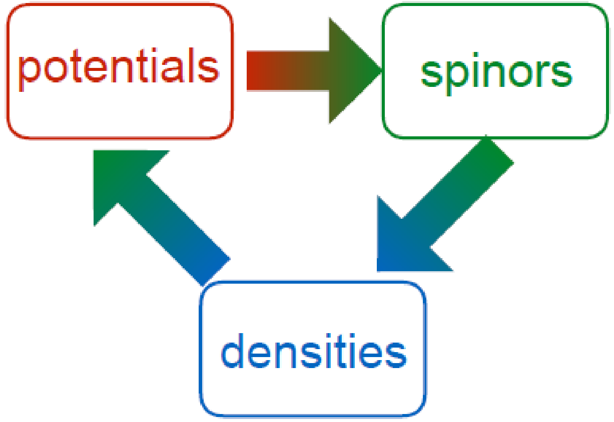
Zhao, ZPLi, Yao & Meng, PRC 2010

- **Single particle Dirac equation:**

$$
\begin{pmatrix} m + V + S & \sigma\cdot p \\ \sigma\cdot p & -(m - V - S) \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix} = \varepsilon \begin{pmatrix} f \\ g \end{pmatrix}
$$

Scalar potential and vector potential

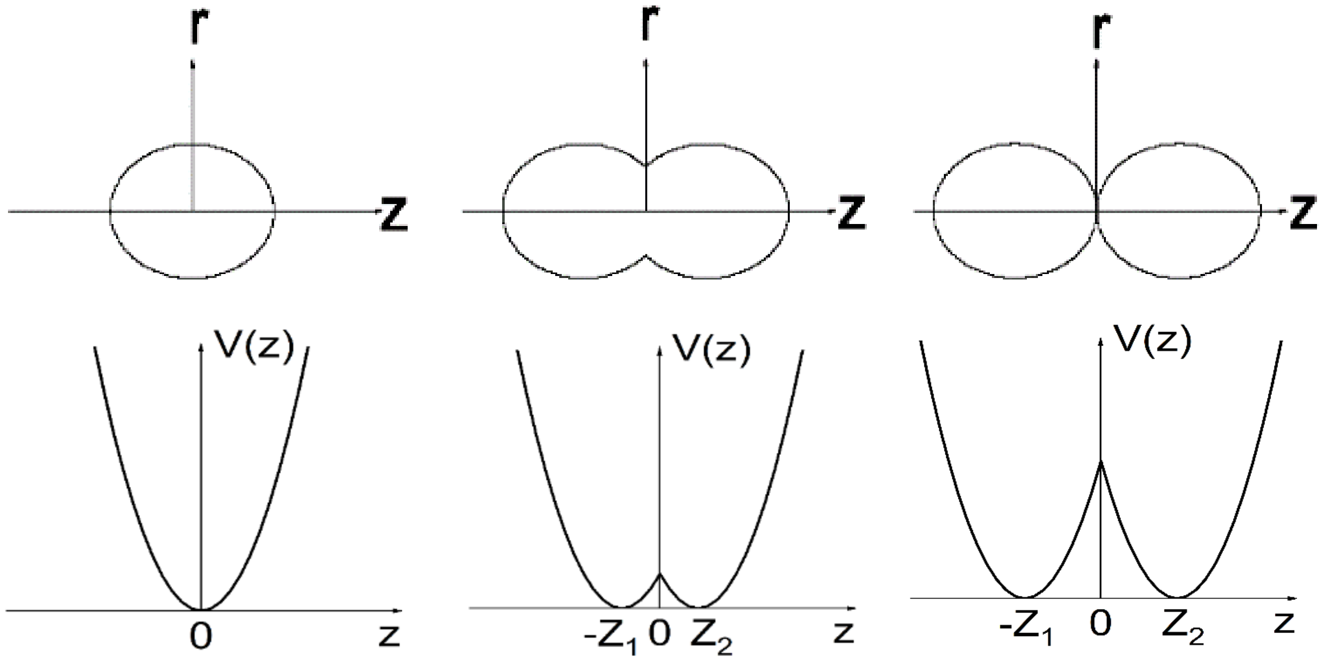
$$
\begin{aligned}
S(\boldsymbol{r}) &= \alpha_S\rho_S + \beta_S\rho_S^2 + \gamma_S\rho_S^3 + \delta_S\triangle\rho_S, \\
V^\mu(\boldsymbol{r}) &= \alpha_V j^\mu + \gamma_V(j_\nu j^\nu) j^\mu + \delta_V\triangle j^\mu - eA^\mu\frac{1-\tau_3}{2} \\
&\quad + \tau_3\left(\alpha_{TV} j^\mu_{TV} + \delta_{TV}\triangle j^\mu_{TV}\right),
\end{aligned}
$$

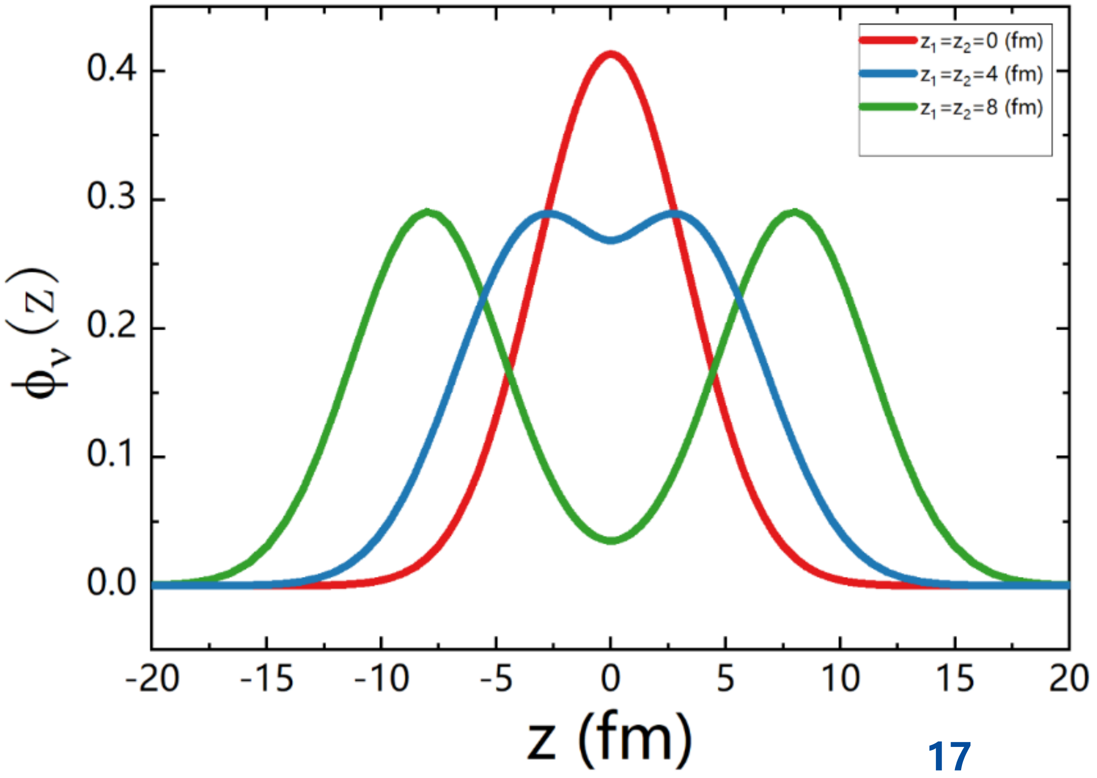


Two Center Harmonic Oscillator basis

➢ **Potential of Two Center Harmonic Oscillator (TCHO) basis**

$$V(r_\perp, z) = V(r_\perp) + V(z) = \frac{1}{2} M\omega_\perp^2 r_\perp^2 + \begin{cases} \frac{1}{2} M\omega_1^2 (z+z_1)^2, & z<0, \\ \frac{1}{2} M\omega_2^2 (z-z_2)^2, & z \geq 0, \end{cases} \xrightarrow[\text{WF}]{\text{Eigen}} \Phi(z, r_\perp, \varphi) = \phi_\nu(z)\phi_{n_r}^{m_l}(r_\perp)\Theta(\varphi)\chi_{m_s}$$





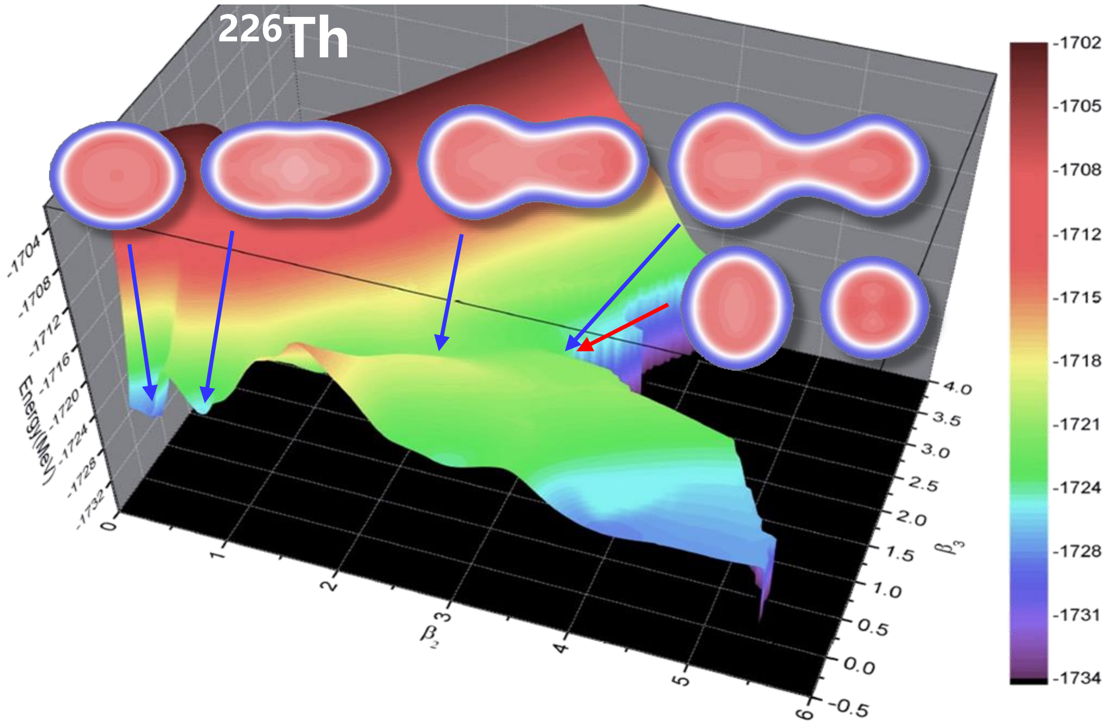
Li, Chen, Zhou, Chen & ZPLi, PRC**109**, 064310 (2024)

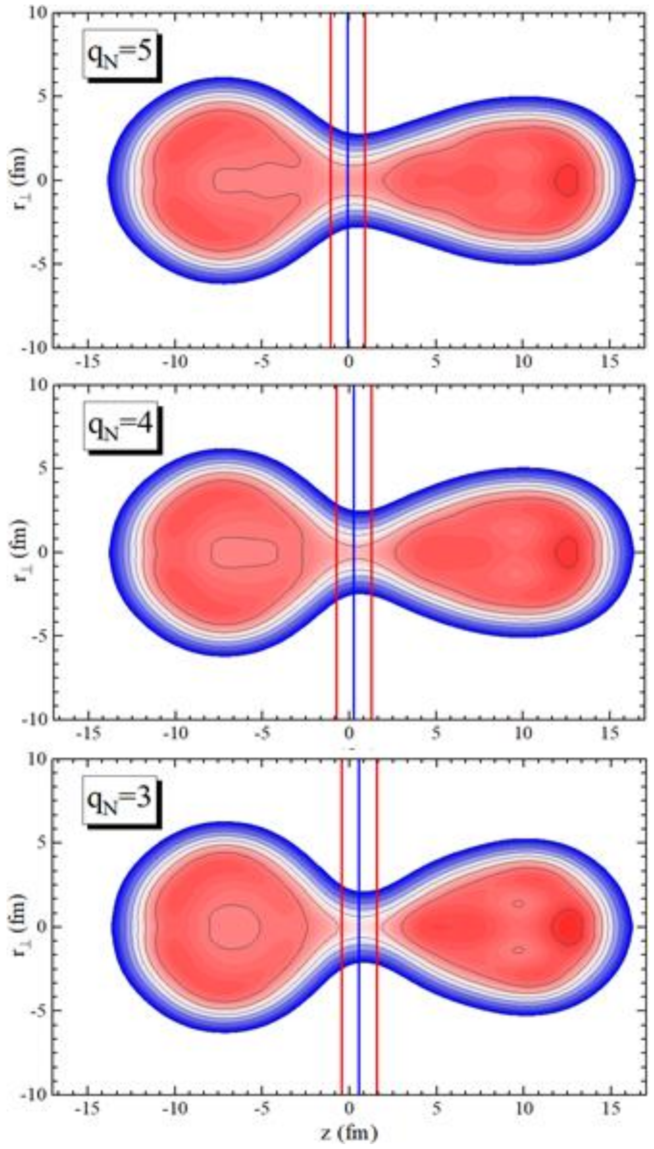
Multi-dimensional constraints for PES

$$\langle E_{RDFT} \rangle + \sum_{k=2,3} C_k(\langle \hat{Q}_k \rangle - q_k)^2 + C_N(\langle \hat{Q}_N \rangle - q_N)^2$$

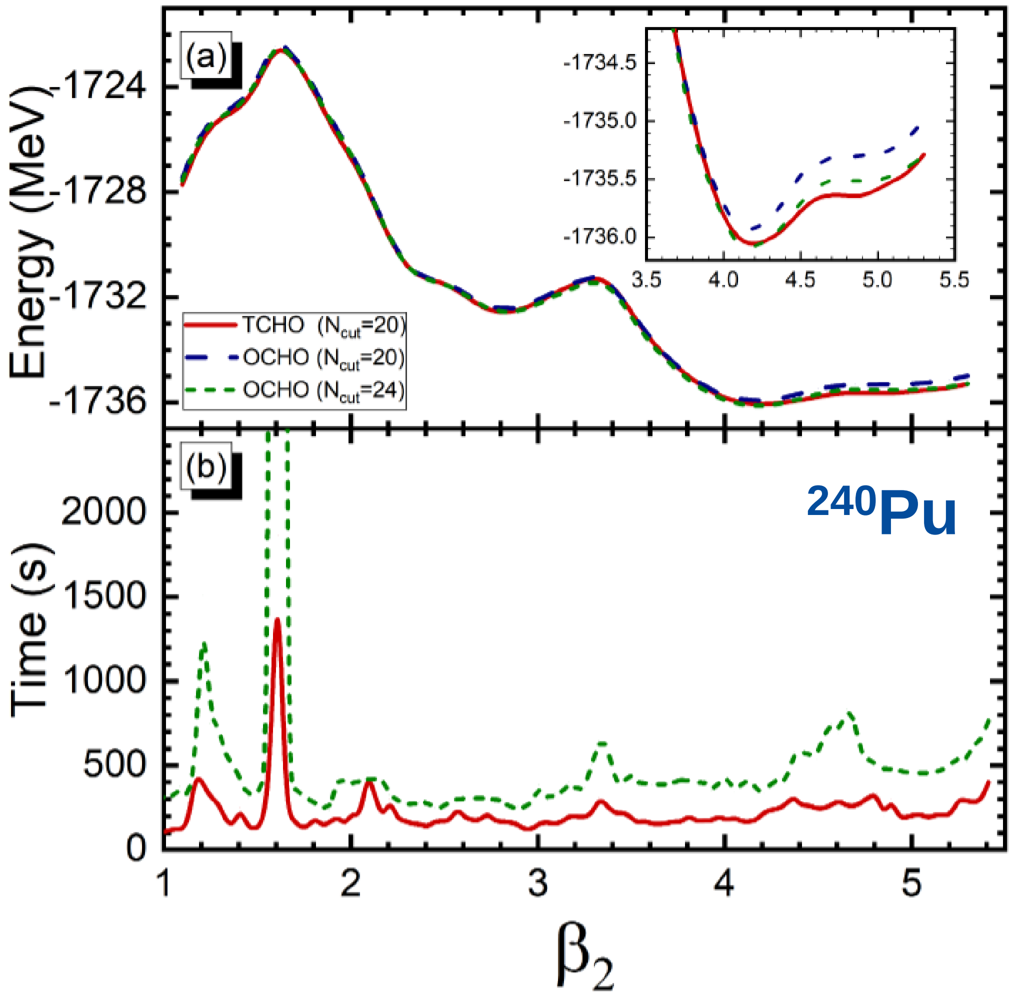
$\hat{Q}_{2,3}$ — **Quadrupole, octupole moment operator**

$\hat{Q}_N = exp[-(z - z_N)^2/a_N^2]$ z_N is the neck, $a_N = 1fm$





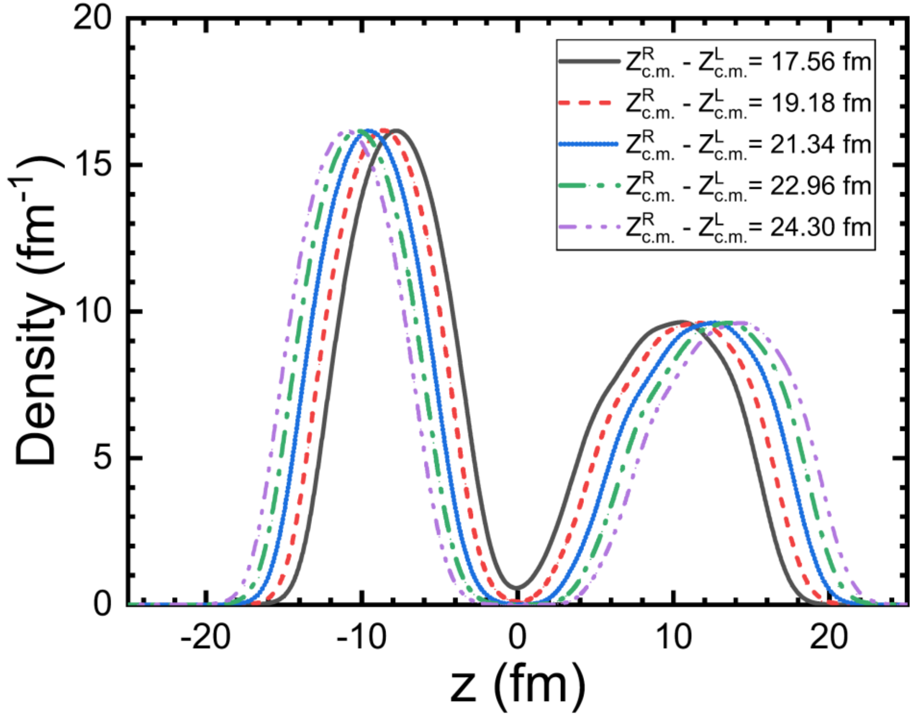
Advantages of RDFT-TCHO



➤ **Better accuracy and efficiency**

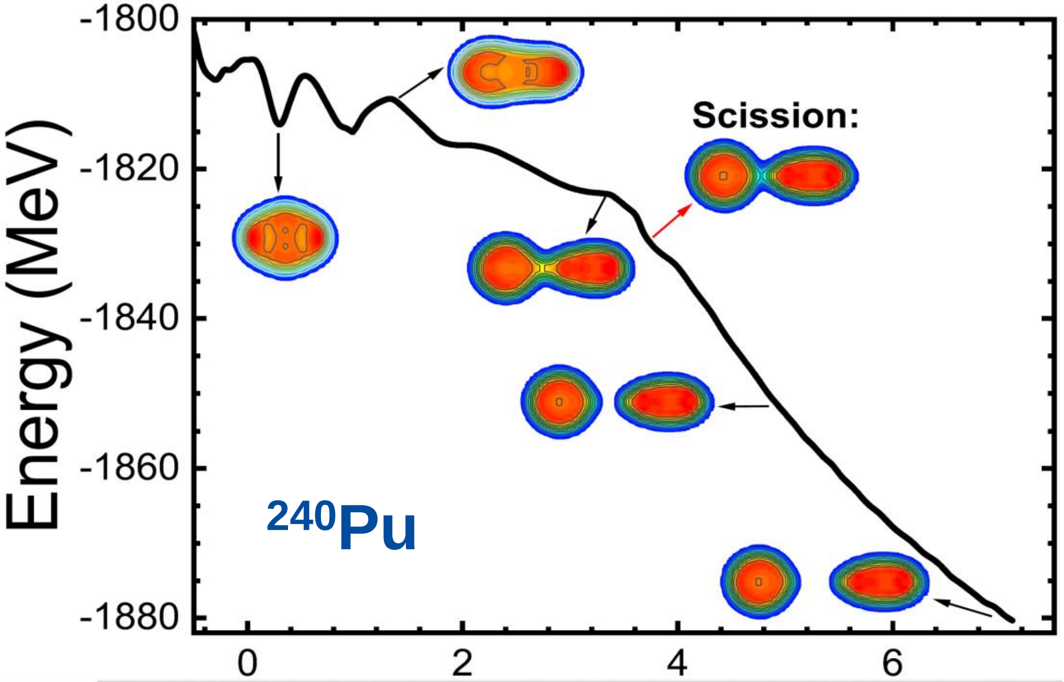
➤ **ρ constraint for post-scission**

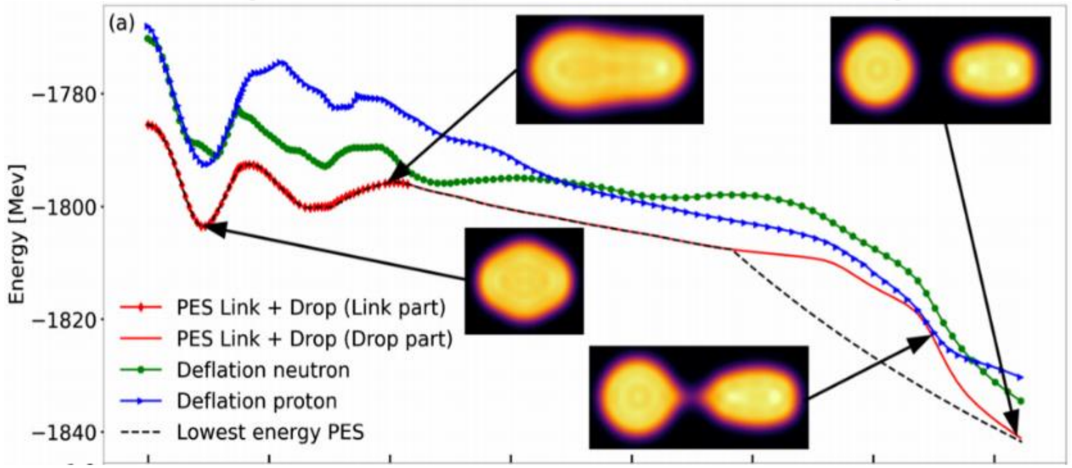
$$\langle E_{\mathrm{tot}}\rangle + C_\rho\left(\int \rho(r_\perp, z) - \rho_0(r_\perp, z)dr\right)^2$$



Li, Chen, Zhou, Chen, ZPLi, PRC109, 064310 (2024)

Advantages of RDFT-TCHO





Q_2

Carpentier, Pillet, Lacroix, Dubray, Regnier, PRL2024

- **Mass tensor calculated in cranking approximation:**

$$\mathcal{B} = \mathcal{M}_{(1)}^{-1}\mathcal{M}_{(2)}\mathcal{M}_{(1)}^{-1}$$

$$\mathcal{M}_{(n),kl} = \sum_{i,j} \frac{\langle i|\hat{Q}_k|j\rangle\langle j|\hat{Q}_l|i\rangle}{(E_i+E_j)^n}(u_i v_j + v_i u_j)^2$$

Girod & Grammaticos, NPA330, 40 (1979)

Provides the microscopic inputs for the dynamical study involving pre-post-scission configurations.

Fission dynamics

➢ **Time Dependent Generator Coordinate Method (TDGCM+GOA)**

$$i\hbar\frac{\partial}{\partial t}g(\beta_2,\beta_3,t)=\left[-\frac{\hbar^2}{2}\sum_{kl}\frac{\partial}{\partial\beta_k}B_{kl}(\beta_2,\beta_3)\frac{\partial}{\partial\beta_l}+V(\beta_2,\beta_3)\right]g(\beta_2,\beta_3,t)$$

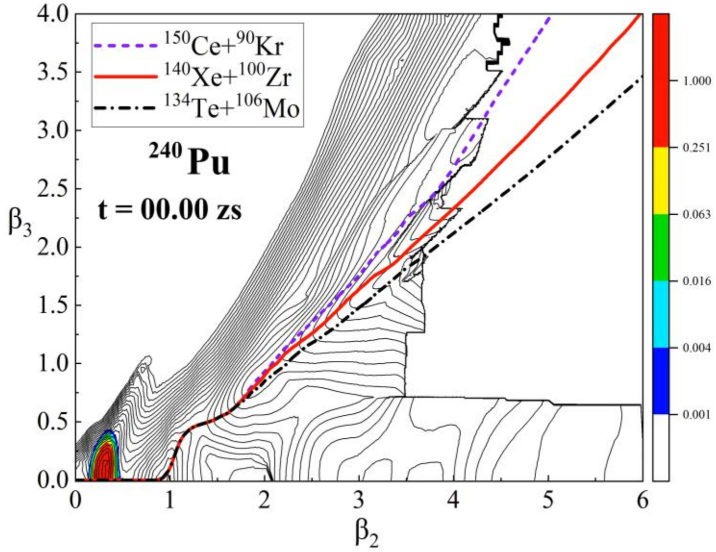
➢ **Probability current**

$$J_k(\beta_2,\beta_3,t)=\frac{\hbar}{2i}\sum_{l=2}^{3}B_{kl}(\beta_2,\beta_3)\left[g^*(\beta_2,\beta_3,t)\frac{\partial g(\beta_2,\beta_3,t)}{\partial\beta_l}-g(\beta_2,\beta_3,t)\frac{\partial g^*(\beta_2,\beta_3,t)}{\partial\beta_l}\right]$$

➢ **Fission yield distribution**

$$Y(A)=\int_0^T dt\vec{J}(\beta_2,\beta_3,t)\cdot\vec{n}ds$$

Evolution of collective probability density diribution

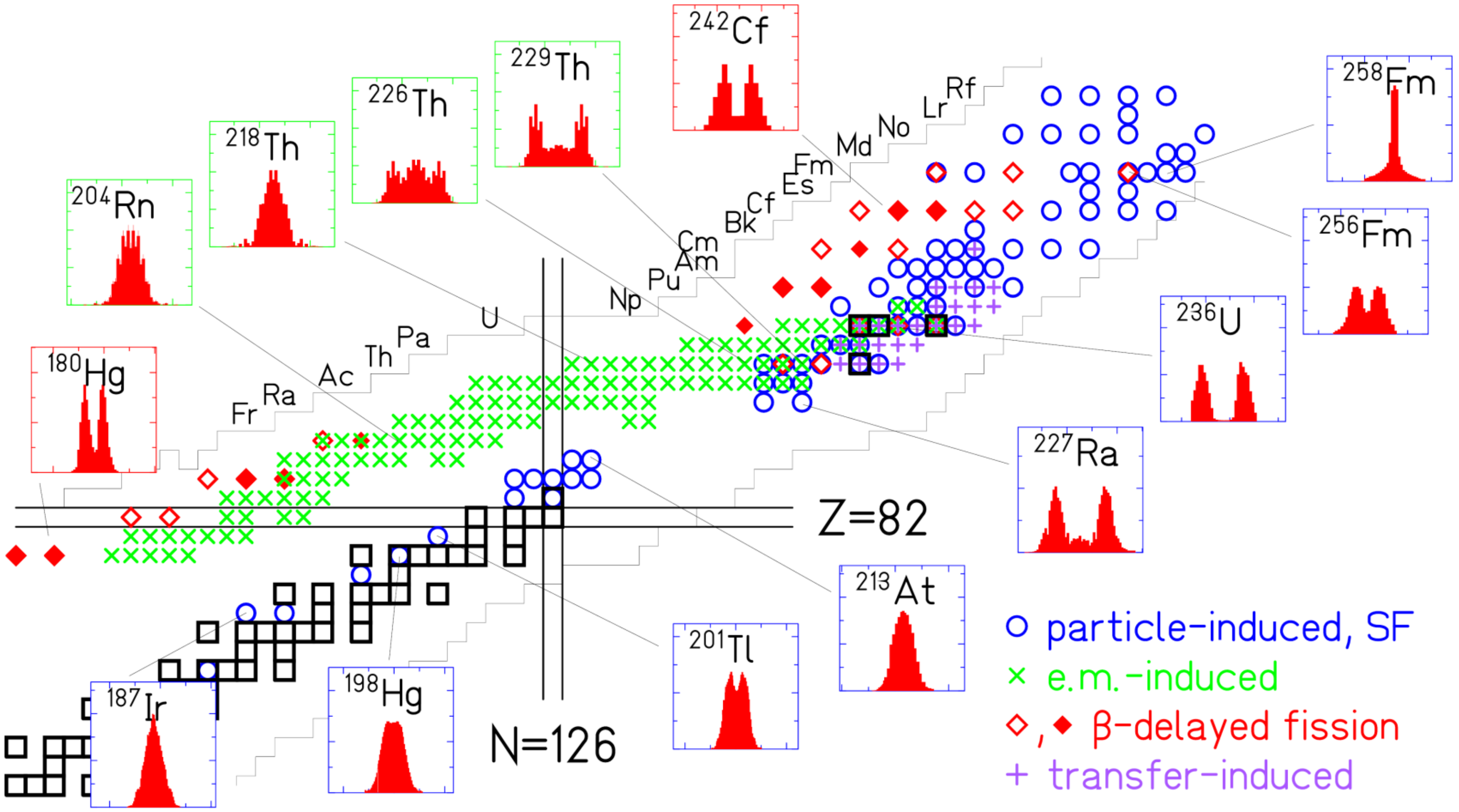


Tao, Zhao, ZPLi, Niksic, Vretenar, PRC96, 024319 (2017)

Result 1

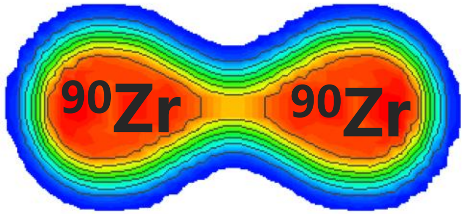
Asymmetric fission of ^{180}Hg

New type asymmetric fission of ^{180}Hg



Andreyev, Nishio & Schmidt, Rep. Prog. Phys. (2018)

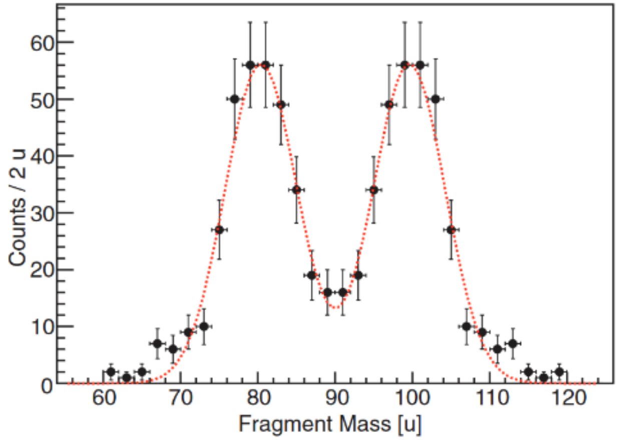
“double magic”



predicted

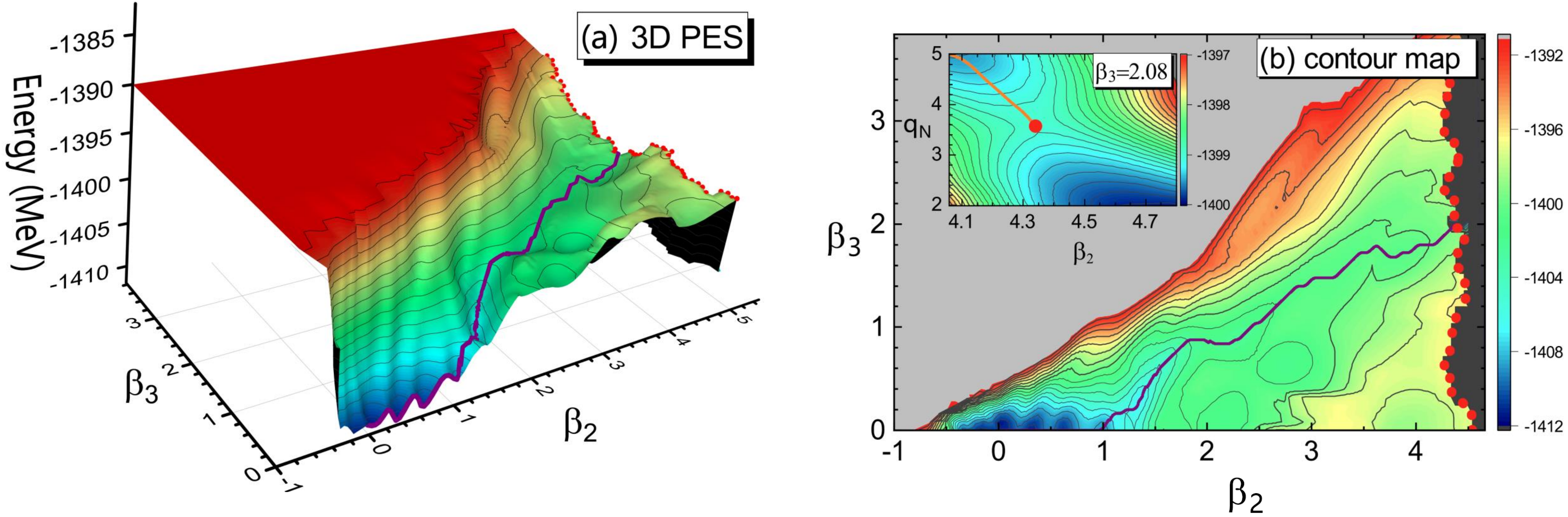
^{180}Hg

observed



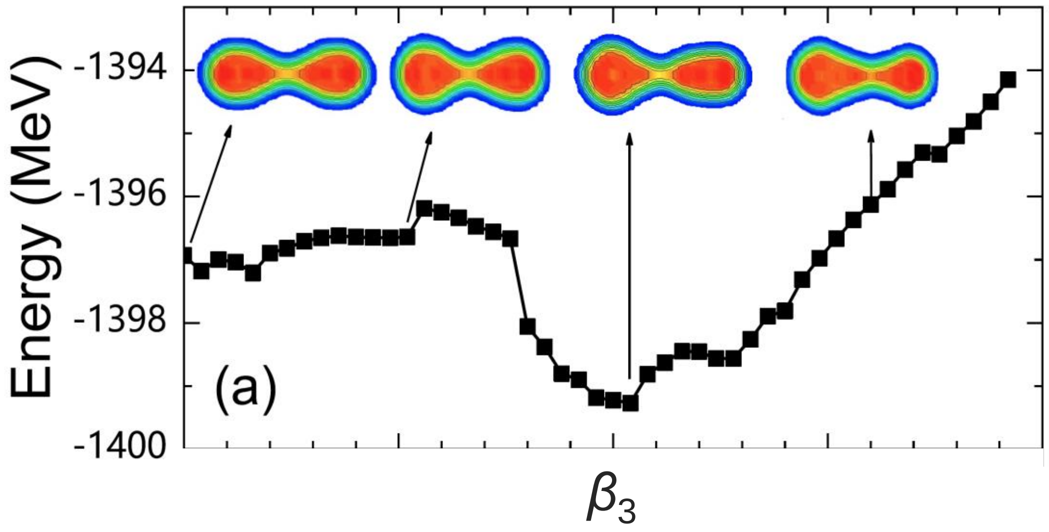
Andreyev et al., PRL (2010)

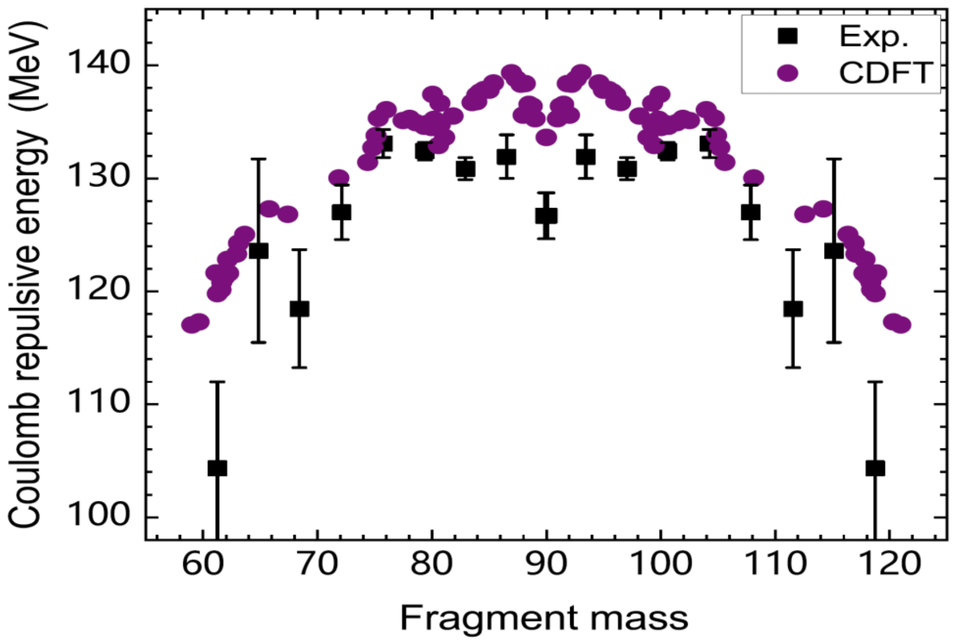
PES of ^{180}Hg

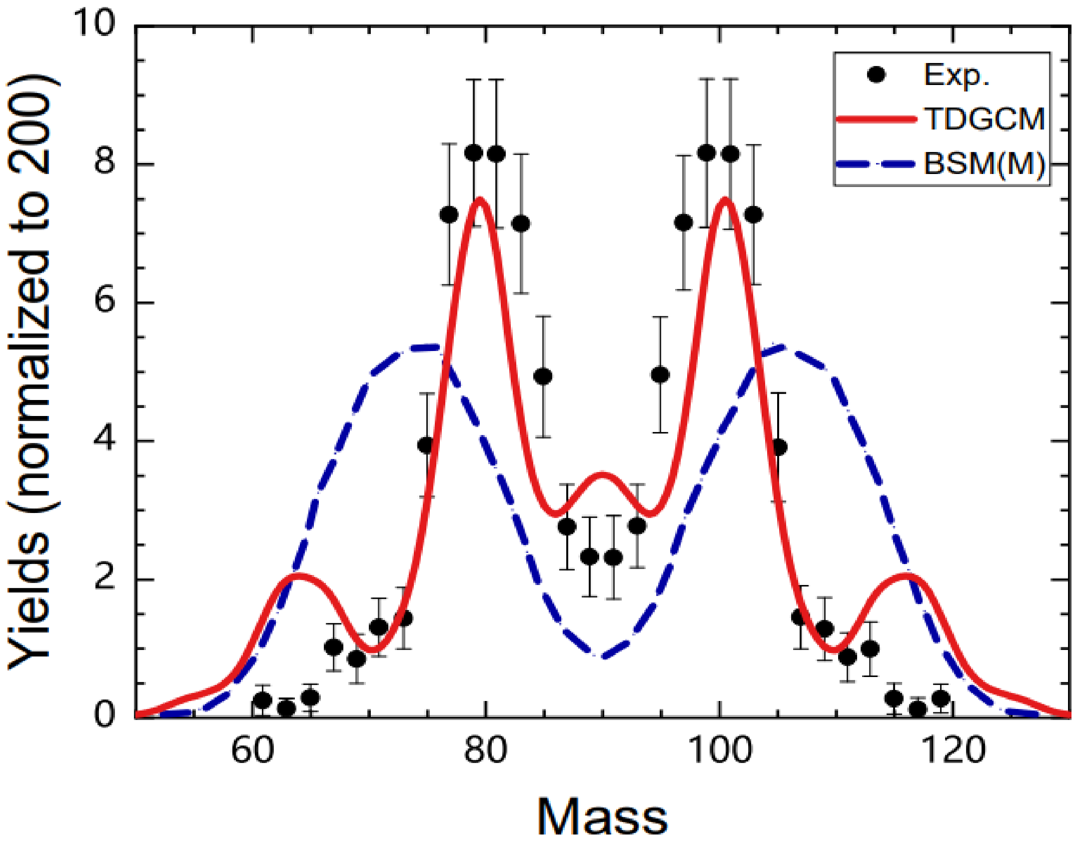


- **Lower asymmetric fission valley is predicted**
- **Scission is defined as the saddle in the β_2-q_N plane**

Scission, TKE, and Yield distributions



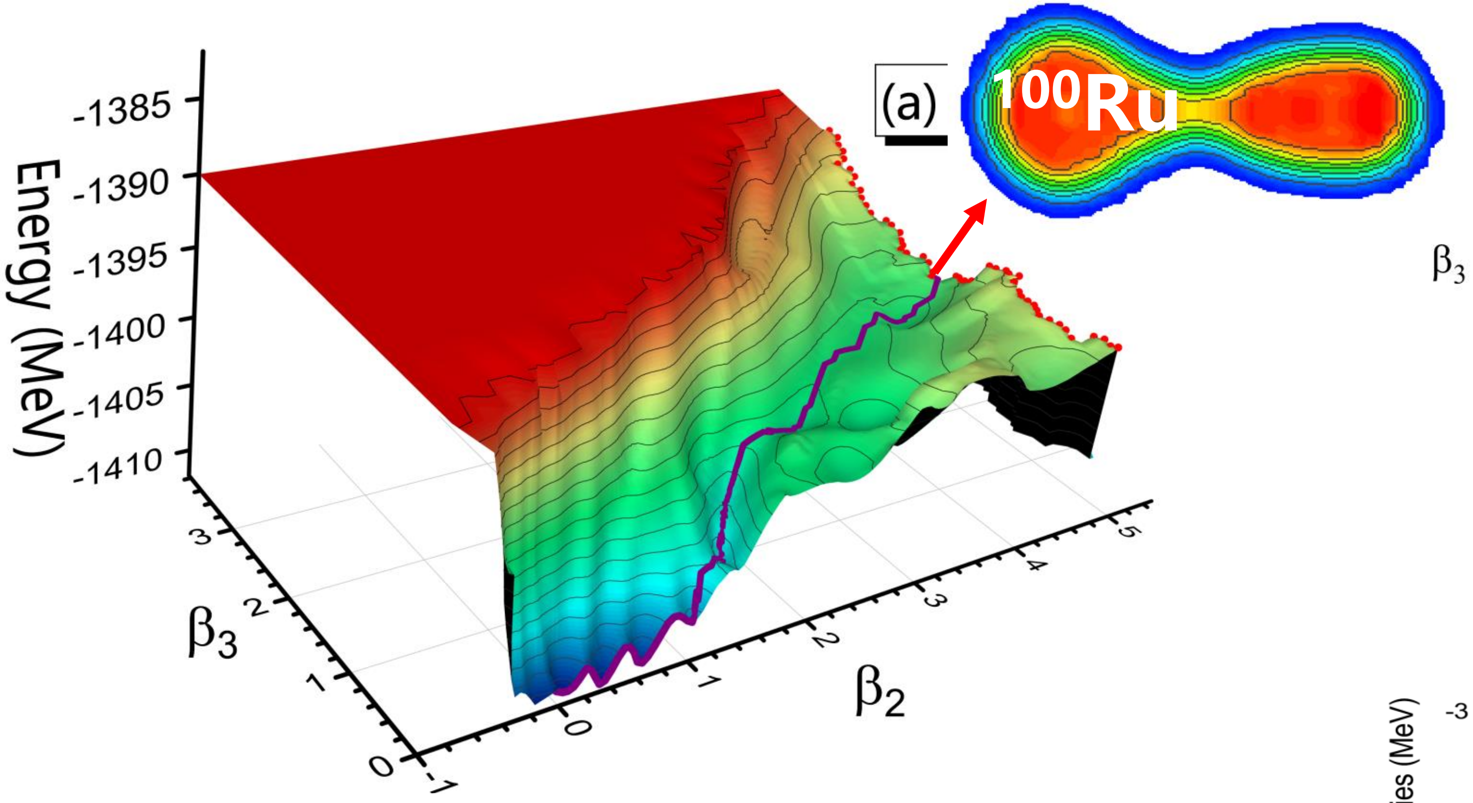


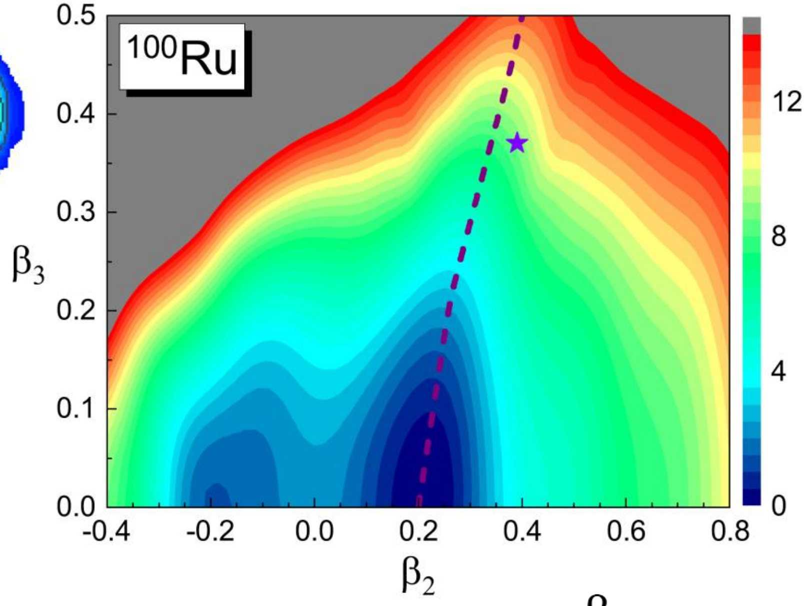


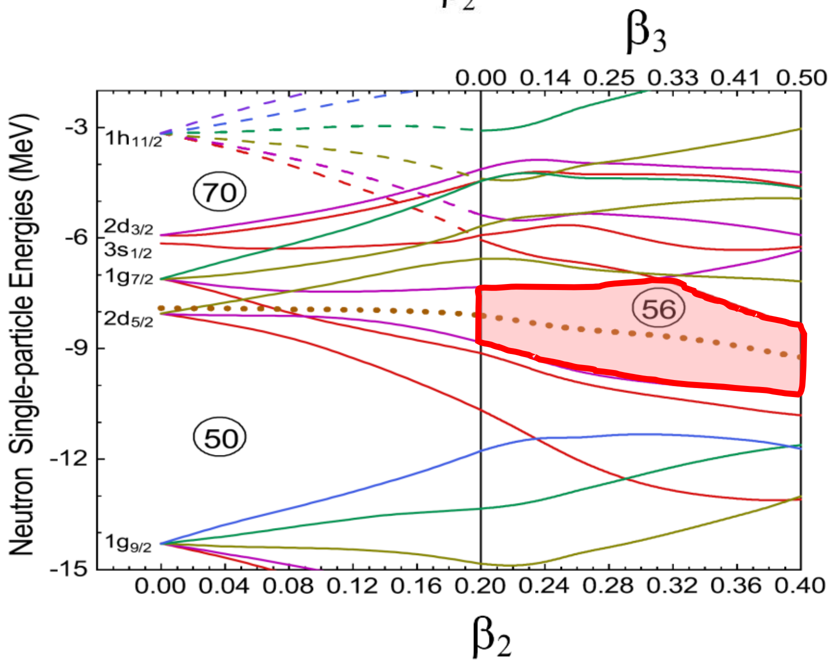
- **Detailed structure of TKE**
- **Reproduce asymmetric fission**

Li, Chen, Chen & ZPLi, PRC 106, 024307 (2022)

Mechanics for asymmetric fission







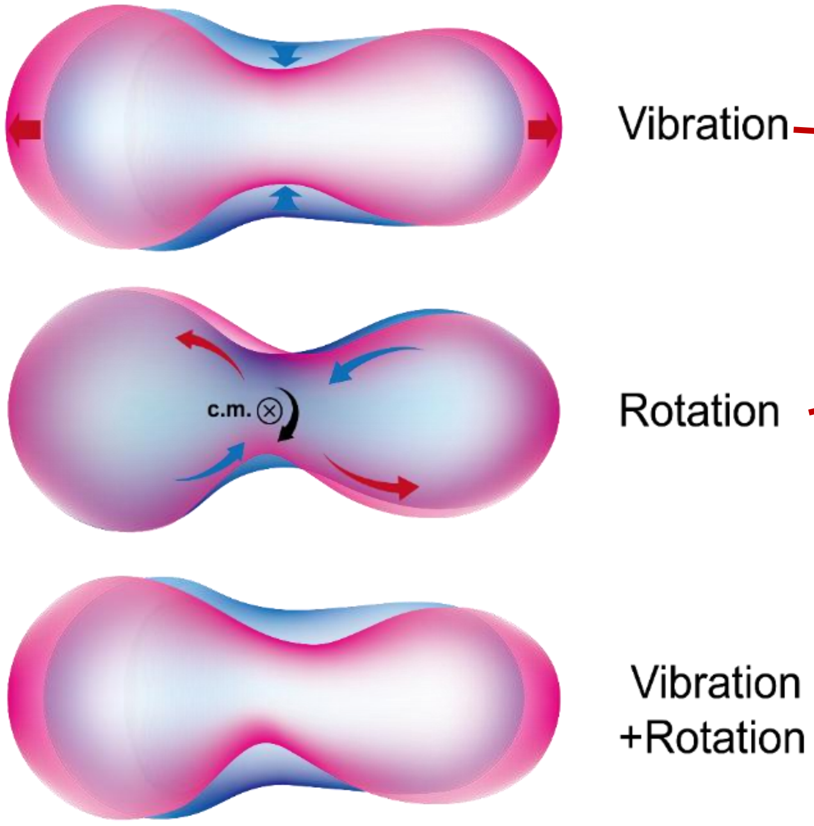
- Heavy fragment ~^{100}Ru: octupole deformed
- N=56 octupole shell of heavy fragment play crucial role

Li, Chen, Chen & ZPLi, PRC 106, 024307 (2022)

Result 2

Fission Fragment Angular Momenta

TD-Multiple Rotations and Vibrations model



Scheme of TD-MRV model

- **Collective Hamiltonian:**

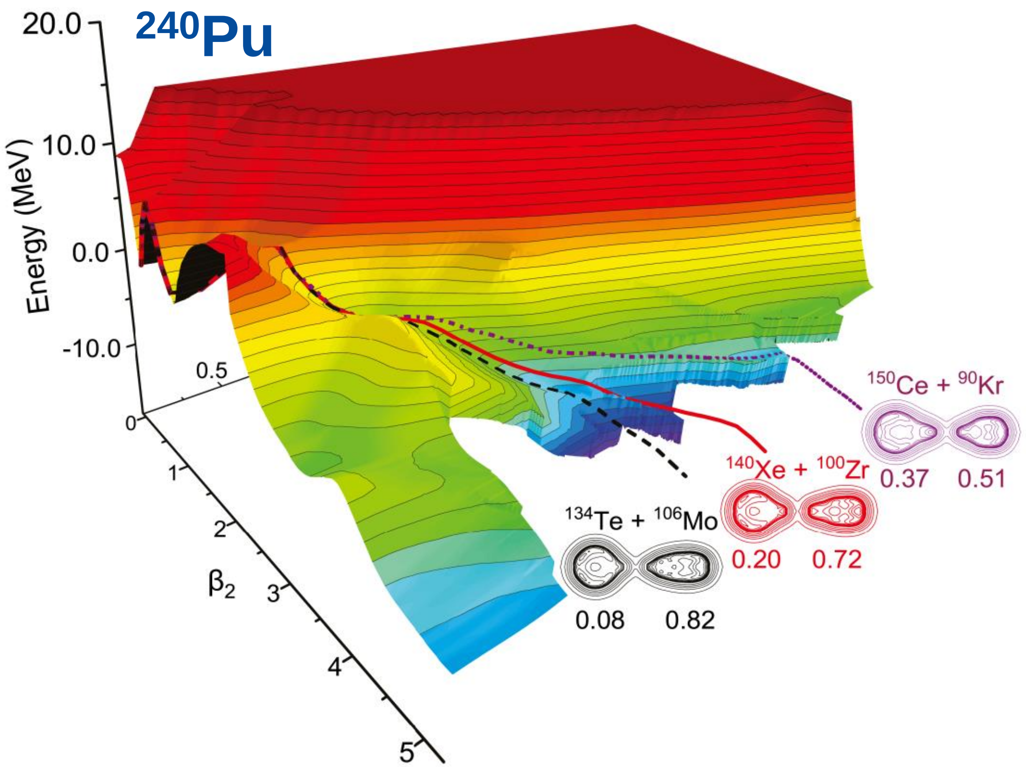
$$\hat{H} = -\frac{\hbar^2}{2}\sum_{p,q=2,3}\frac{\partial}{\partial\beta_p}B^{-1}_{pq}\frac{\partial}{\partial\beta_q} + V(\beta_2,\beta_3) + \sum_i \frac{\hat{S}_i^2}{2\mathcal{I}_i} + \sum_{i<j}\chi_2\hat{Q}_2^i\cdot\hat{Q}_2^j \qquad (i,j = L,\ H,\ \Lambda)$$

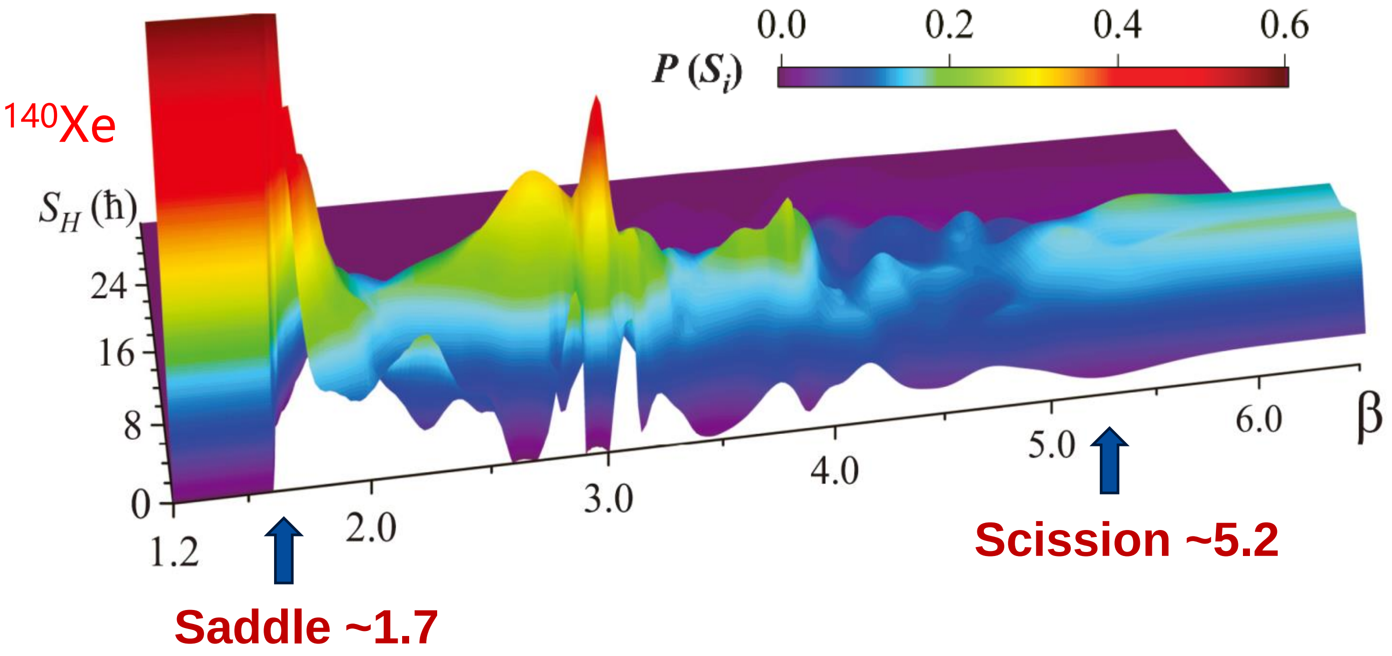
$$\hat{Q}^i_{2\mu} = D^2_{\mu 0}q^i_2 = D^2_{\mu 0}\cdot\frac{3}{4\pi}A_iR_0^2\beta_2^i$$

- **Wave function of the system:**

$$\sum_n \phi_n(\beta_2,\beta_3,t)|S_LS_H(S_{LH})S_\Lambda;JM\rangle \qquad n\equiv(S_L,S_H,S_\Lambda)$$

Evolution of Fragment Angular Momenta (FAM)

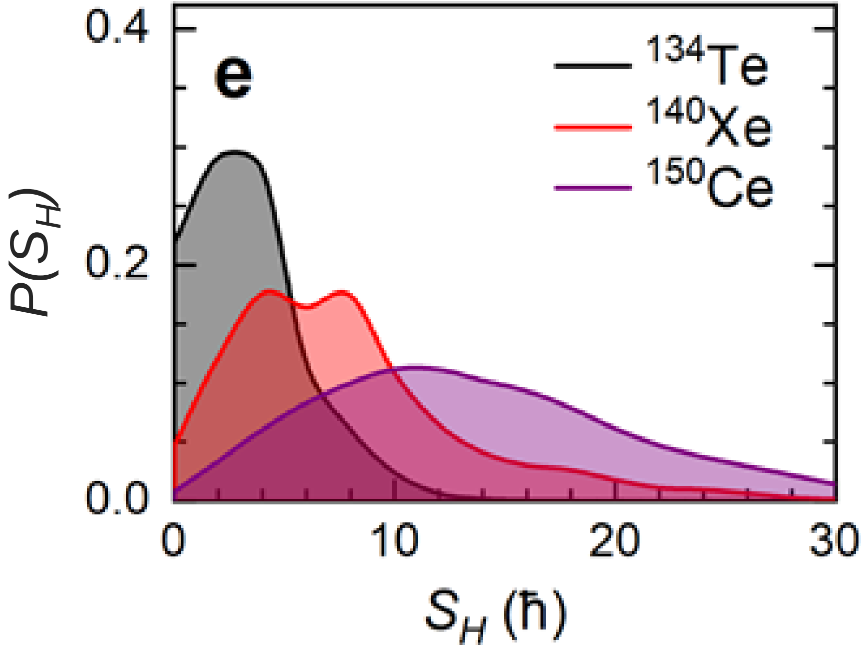


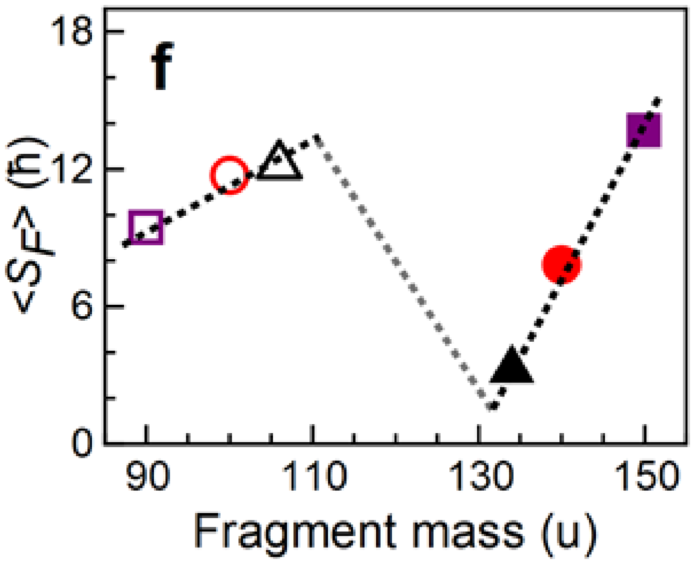


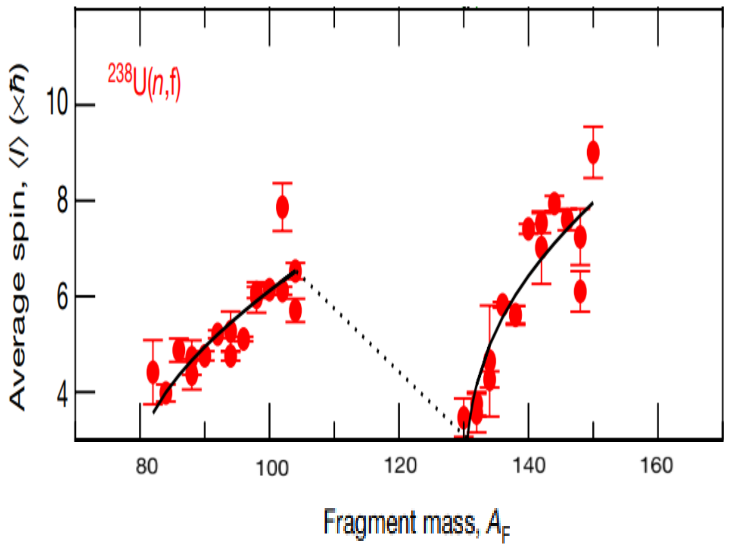
- From saddle to scission: **Rapid generation** and **chaotic evolution** of FAM
- After scission: **Vary slightly till to a stable pattern** when the fragments are well separated.

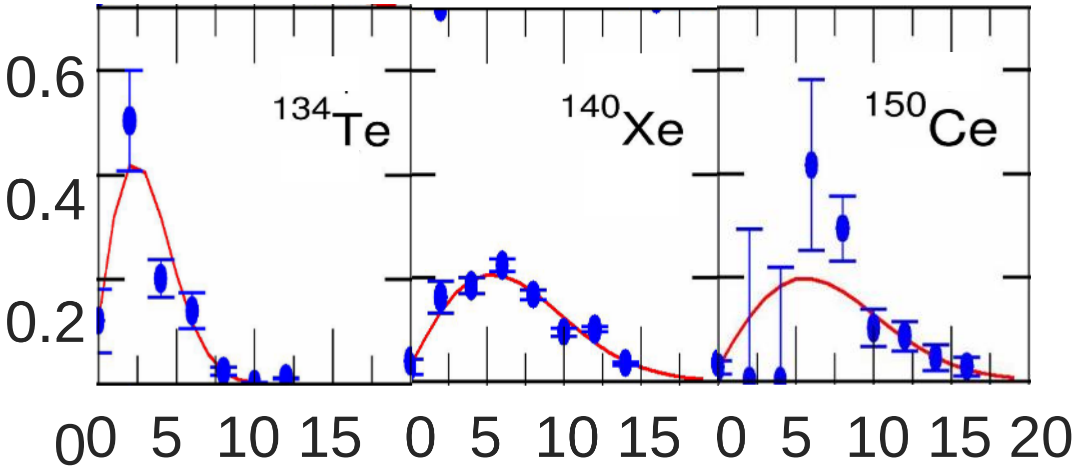
Distributions of FAM

J. N. Wilson, et al., Nature 590, 566 (2021)





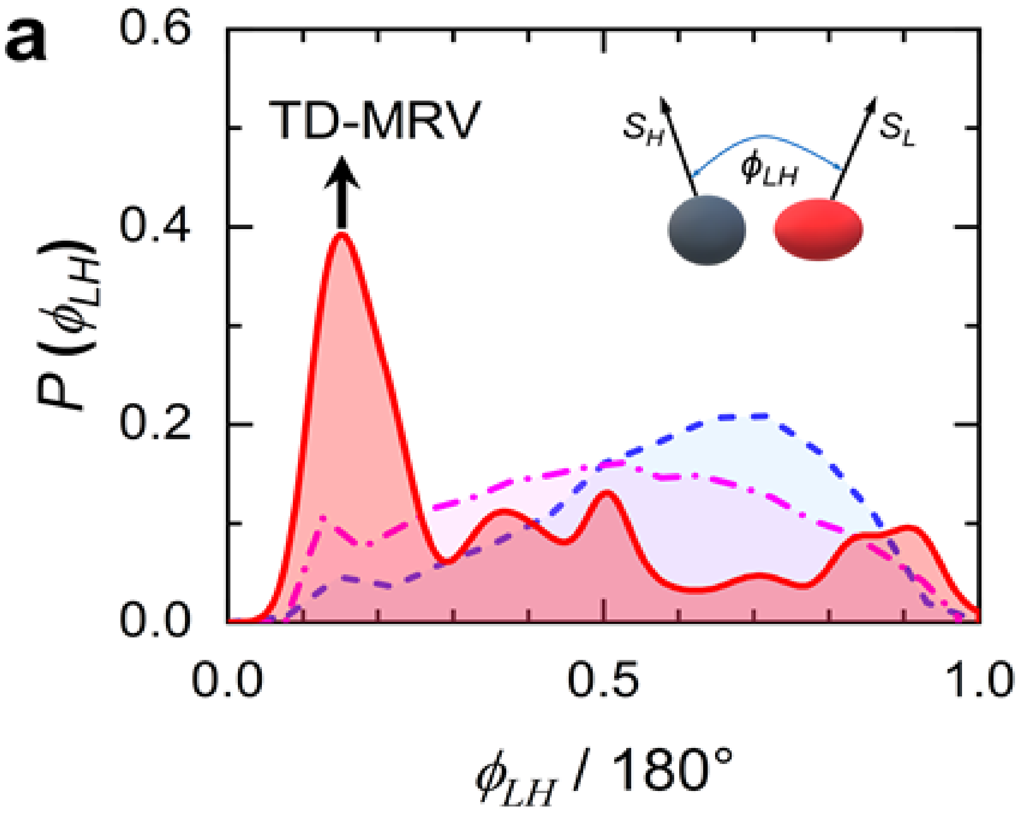


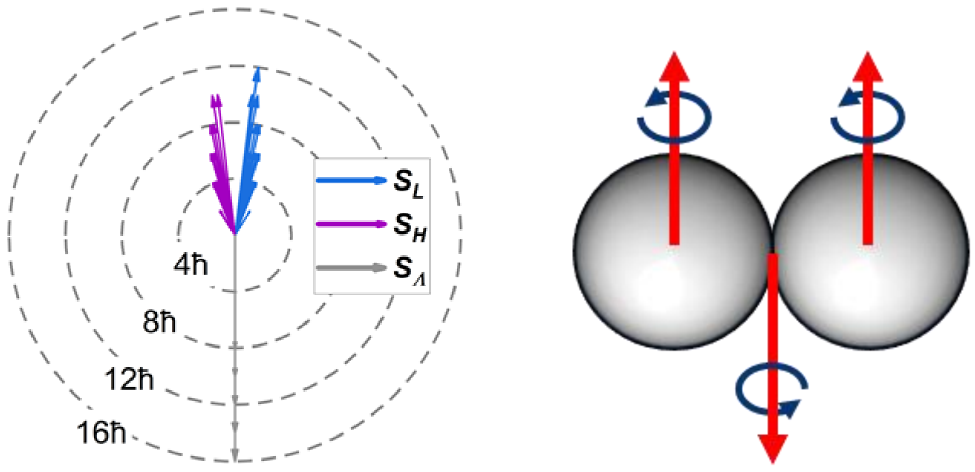


- With the increase of A_F, the $P(S_H)$ increases rapidly: **2ħ~10ħ**.
- The mass dependence of average FAM presents a clear **sawtooth-like pattern**.

Correlations of FAM

Zhou, Chen, Li, Smith & ZPLi, arXiv:2311.06177



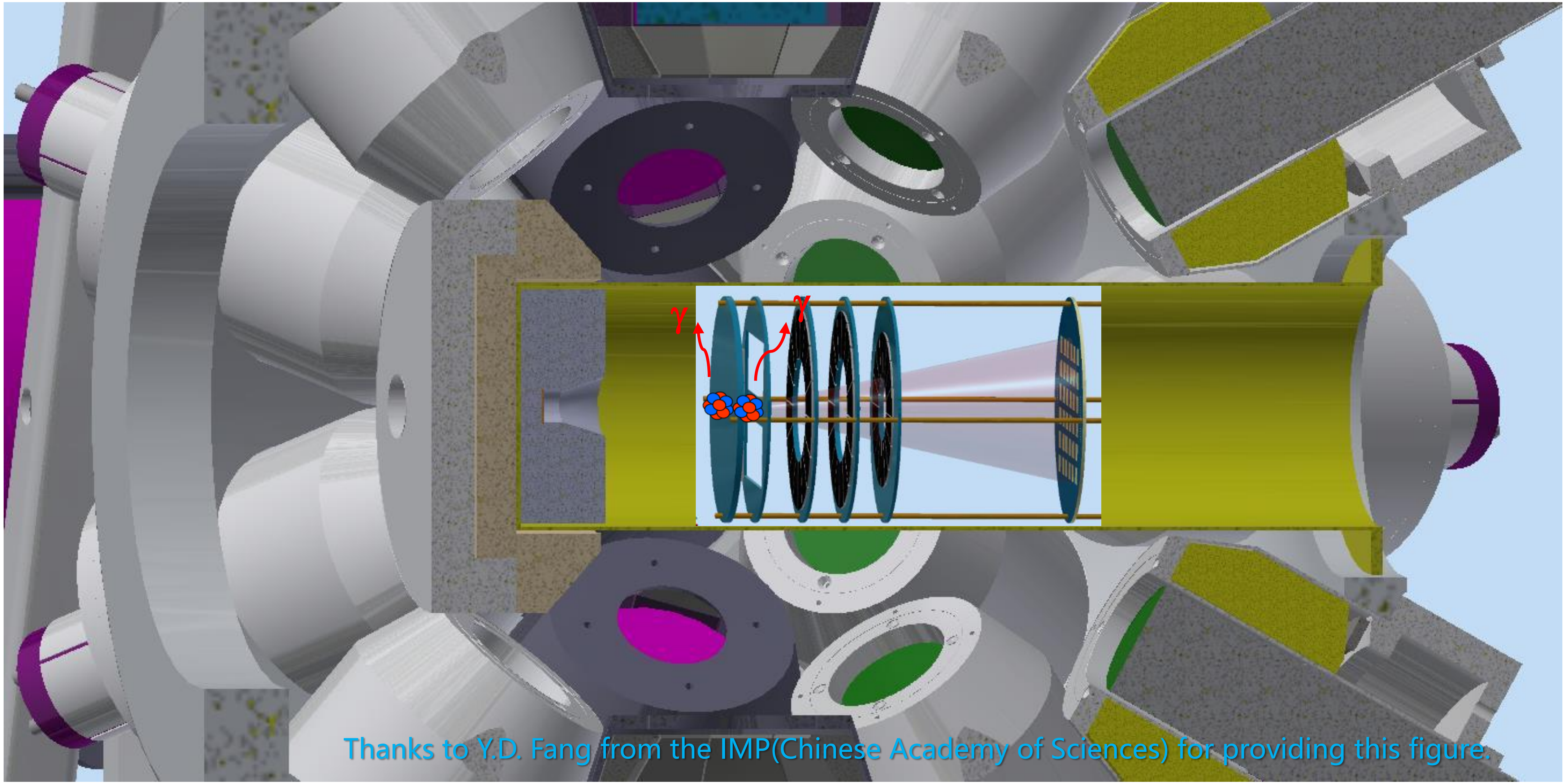


Dominated by **Wriggling mode**

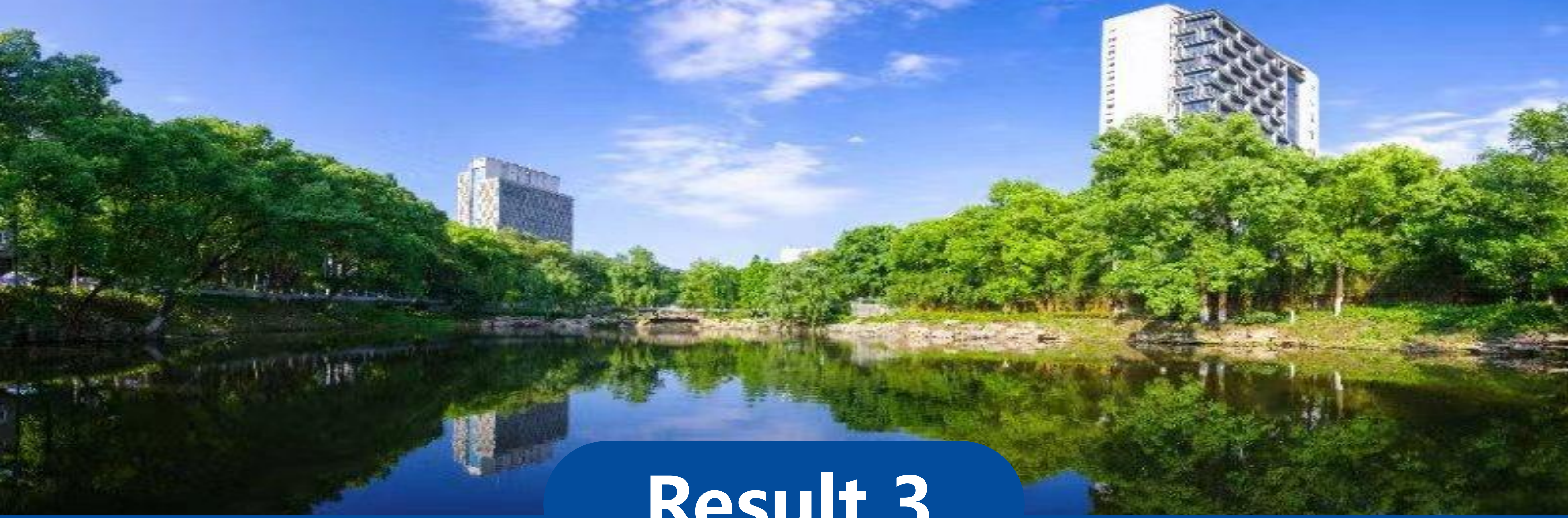
- Opening angle displays strong correlations at **~30°, 90°, and 160°.**
- Differ from those of AMP (blue) and statistical model (magenta), which did not consider quantum shape fluctuations.

Measurement of correlations of FAM

西南大學



We have carried out the experimental measurements for correlations of γ related to FAM from ^{252}Cf source in IMP, Lanzhou, China.

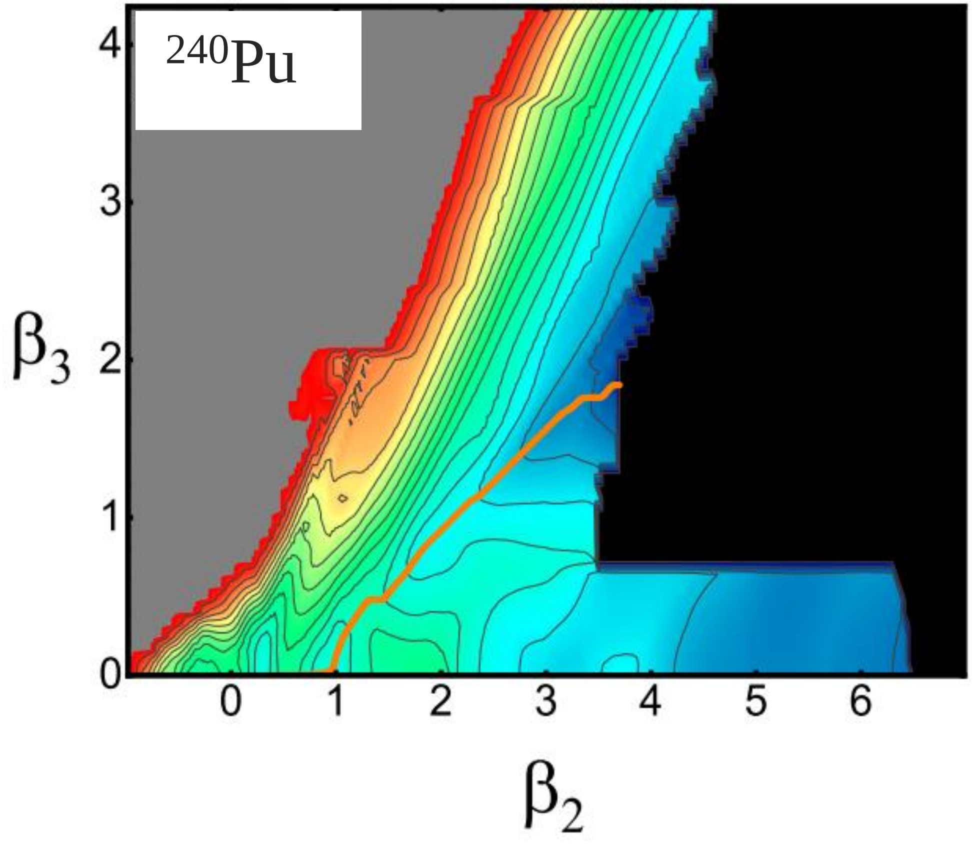


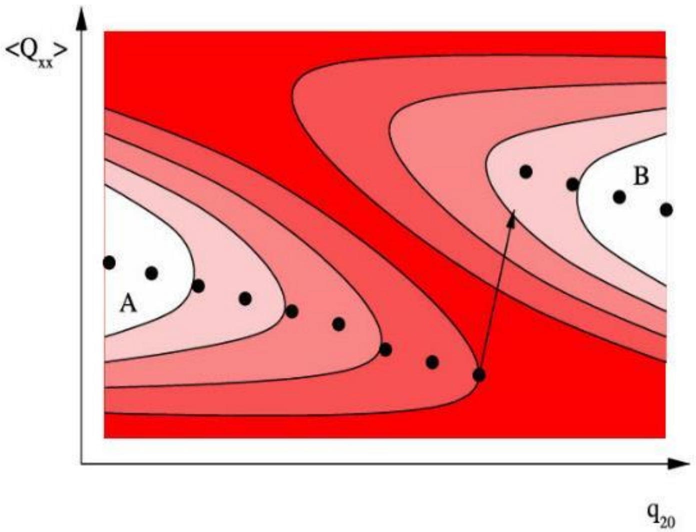
Result 3

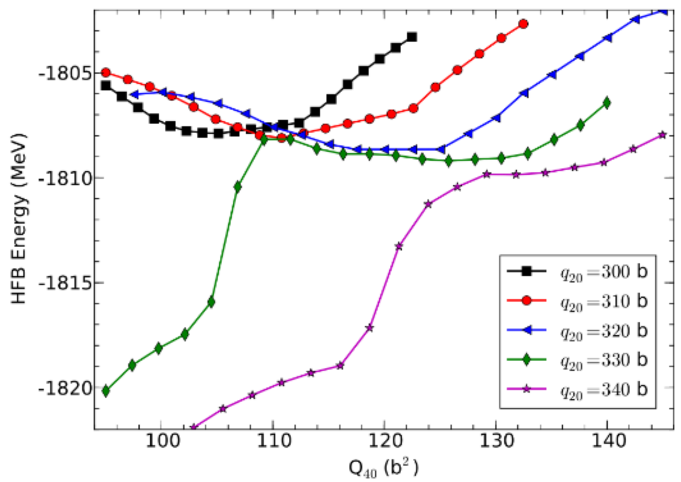
Multi-dimensional collective space

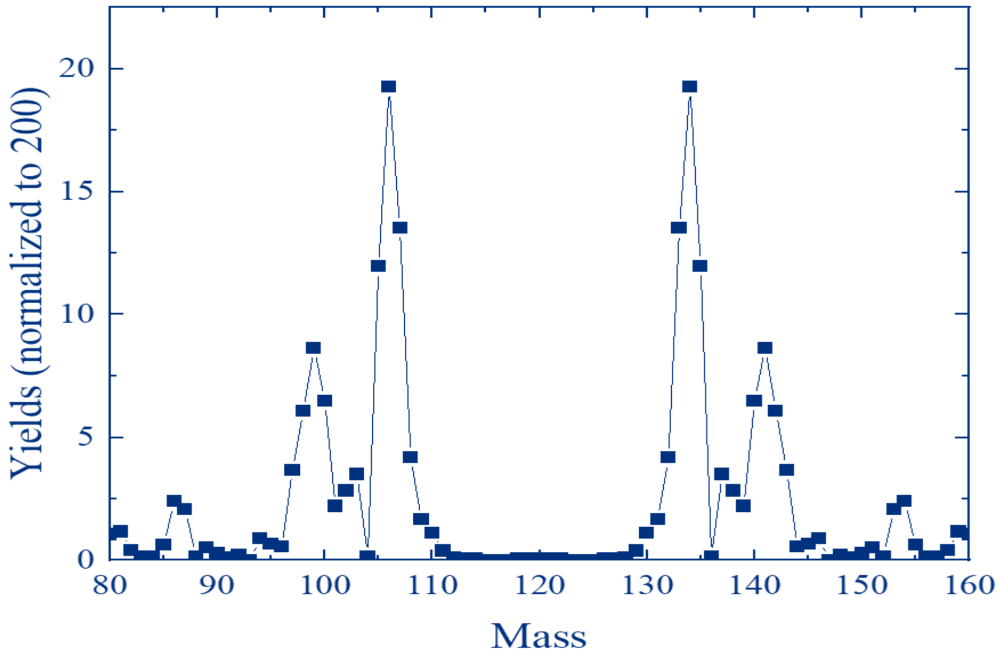
Limitation of 2D space

Discontinuity!







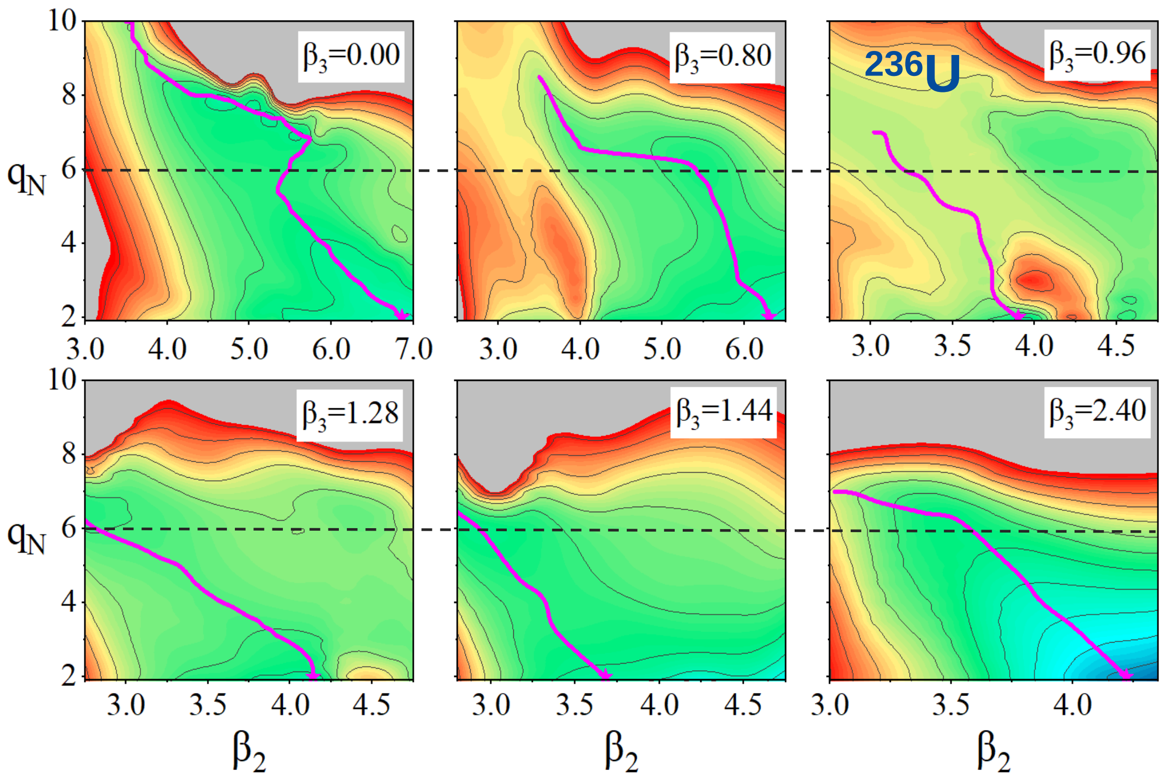


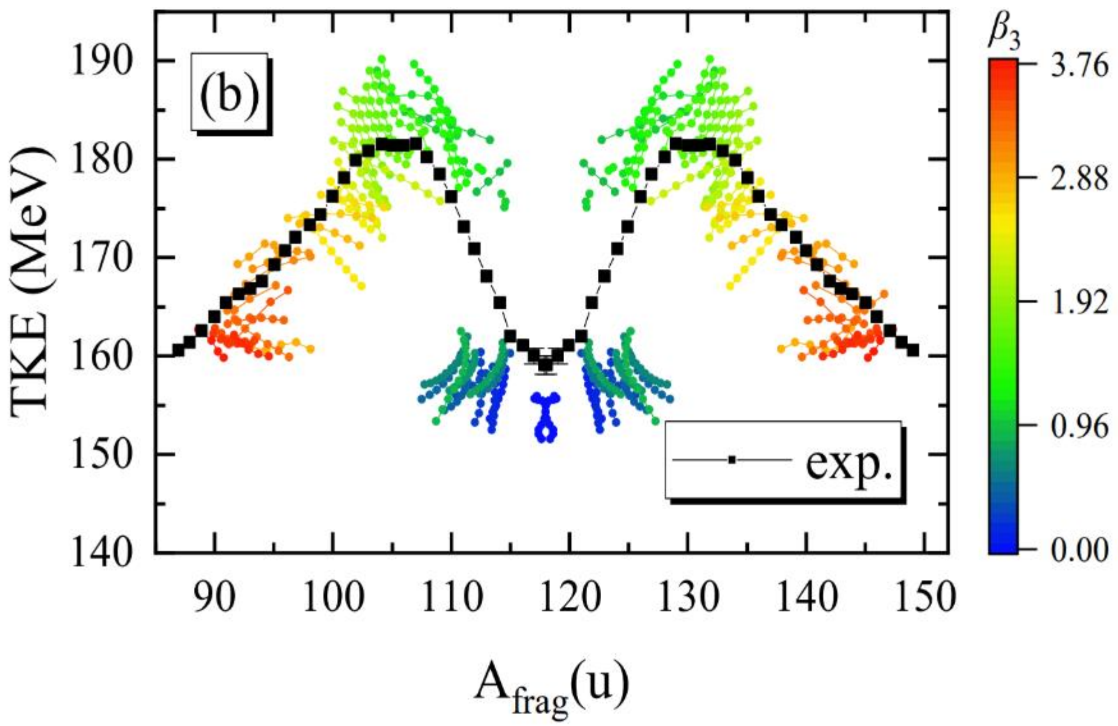
Dubray, Noël & Regnier, CPC2012;

Zdeb, Warda & Robledo, PRC2021;

....

3D PES with nucleon number at neck (q_N)





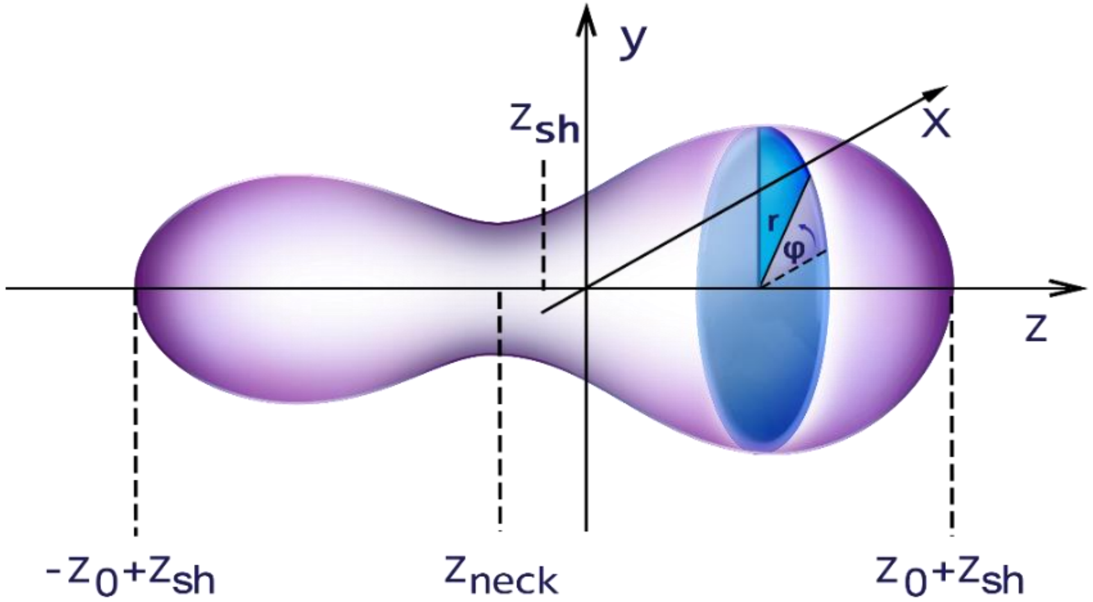
- **q_N<6, PES is very flat: large fluctuations**
- **Coexistence of fission modes**

Zhou, Li, Chen, Chen & ZPLi, Chin. Phys. C (2023)

- **Few to ~10 MeV** fluctuation in TKE
- **Few to ~10 nucleons** fluctuation in A_{frag}

q_N cannot be defined globally!!

Nuclear Shapes in Fourier Expansion



- **Expand r(z, φ) instead of R(θ, φ)**

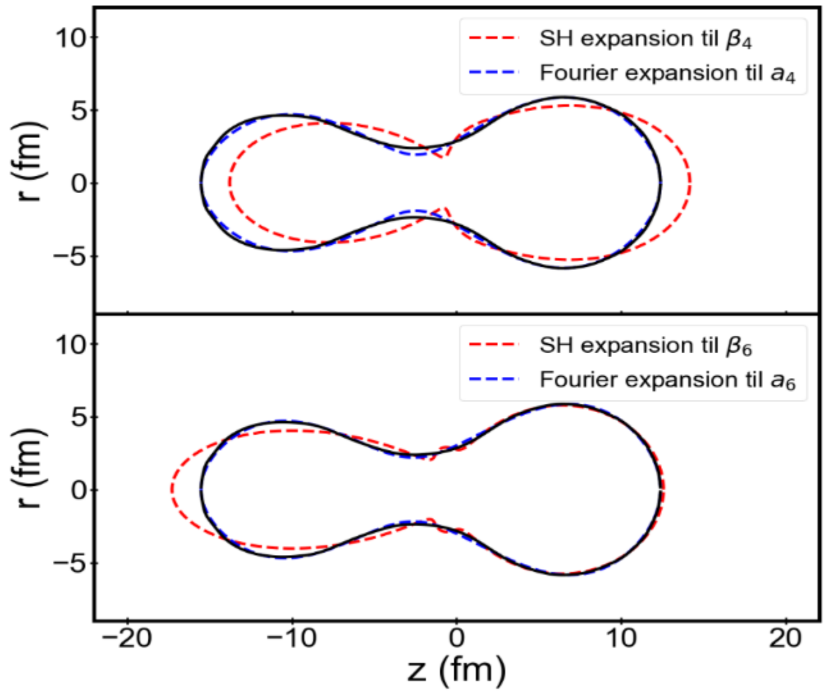
$$r^2(z) = R_0^2 \sum_{n=1}^{\infty} \left[a_{2n} \cos\left(\frac{(2n-1)\pi}{2} \frac{z - z_{sh}}{z_0} \right) + a_{2n+1} \sin\left(\frac{2n\pi}{2} \frac{z - z_{sh}}{z_0} \right) \right]$$

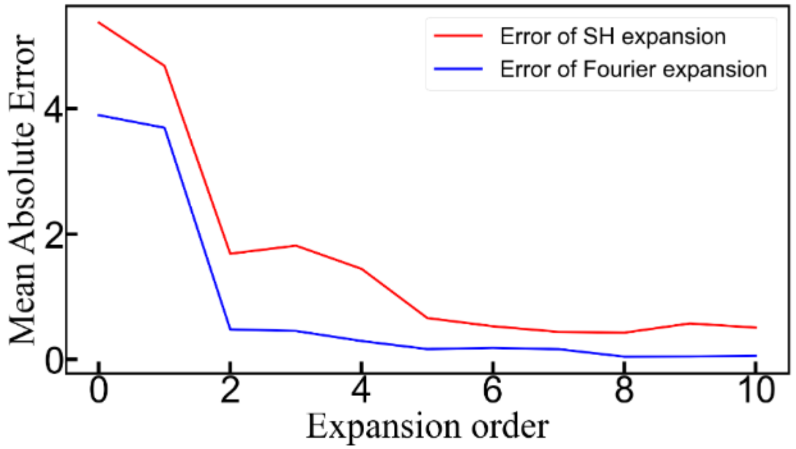
z_0 : Half length of atomic nucleus along z axis

z_{sh}: The geometric center along the z axis

K. Pomorski et al. Acta Phys. Pol. B Supl. 13, 361(2020)

- **Expansion convergency**



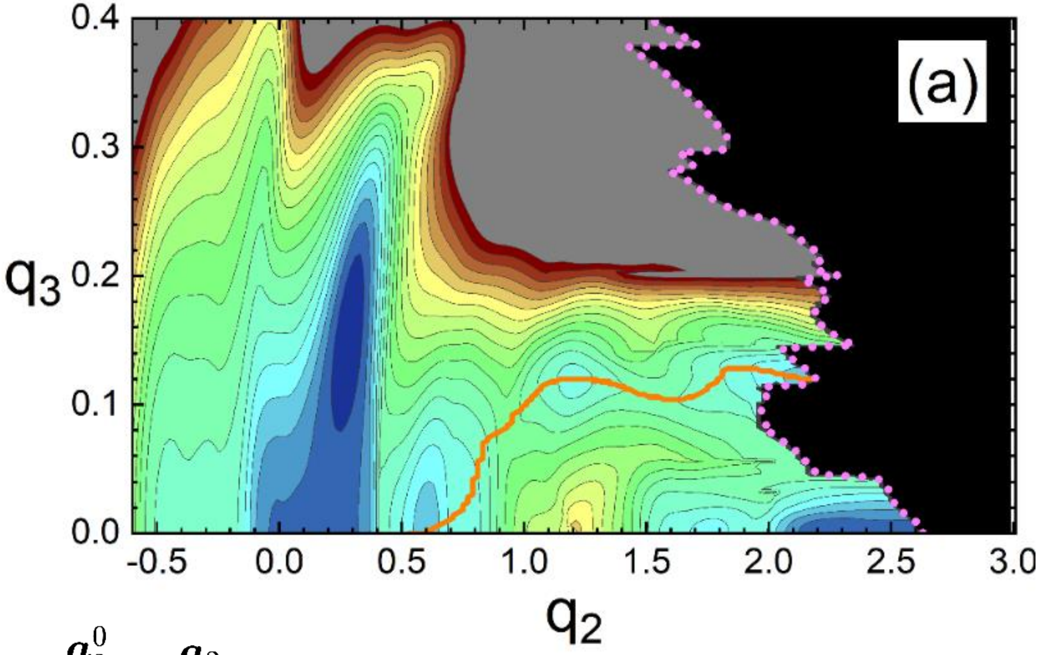


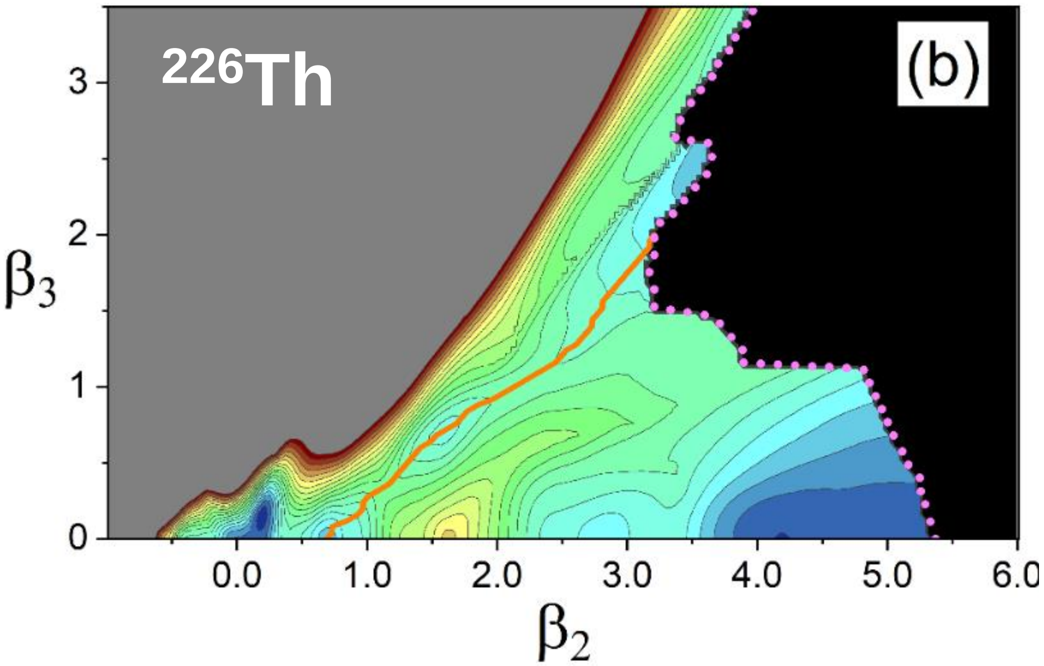
PES in Fourier deformations

$$a_{2n} = \int \frac{4R_0}{3Az_0}\cos\left(\frac{(2n-1)\pi(z-z_{sh})}{2z_0}\right)\rho_{RDFT}(r,z)rdrdz$$

$$a_{2n+1} = \int \frac{4R_0}{3Az_0}\sin\left(\frac{n\pi(z-z_{sh})}{z_0}\right)\rho_{RDFT}(r,z)rdrdz$$

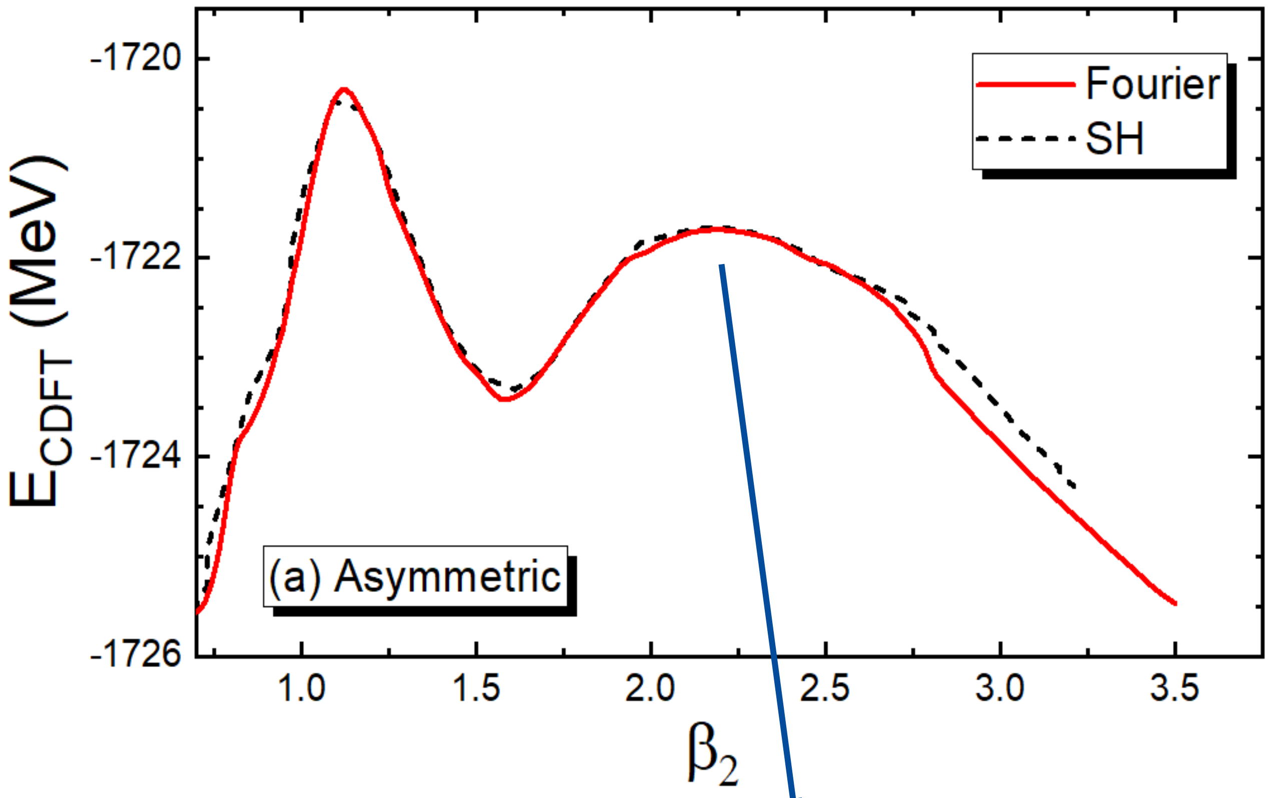
- Deformation operator





$$q_2 = \frac{a_2^0}{a_2} - \frac{a_2}{a_2^0} \quad q_3 = a_3$$

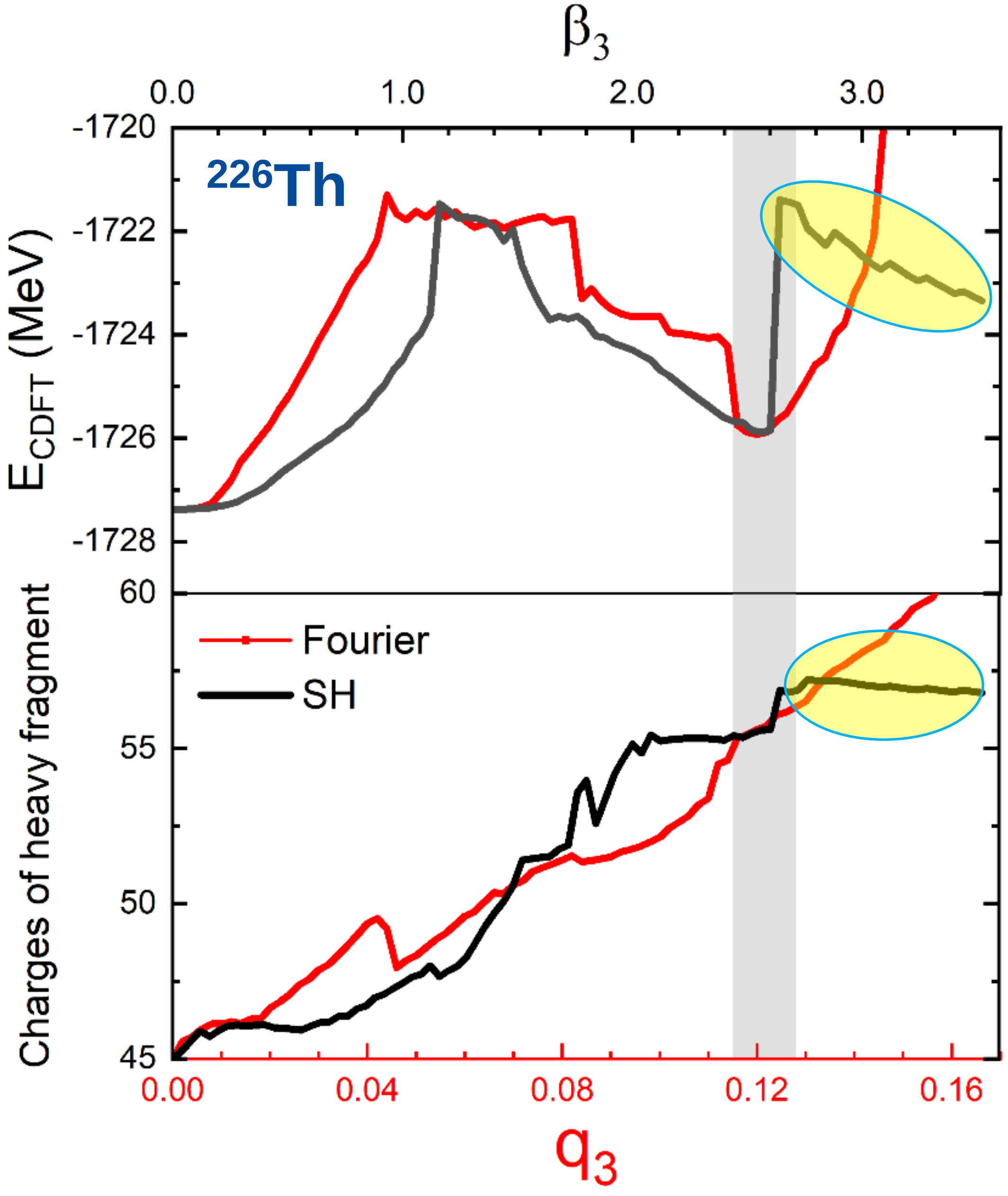
Convergency for expansion orders



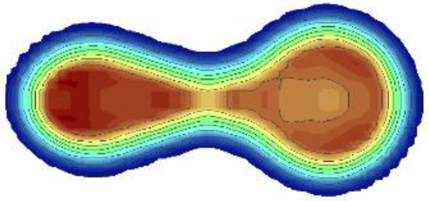
- **Similar PECs before $\beta_2 = 2.5$**
- **More reasonable configurations for larger deformations**

n	2	3	4	5	6	7
a_n	0.4865	0.1050	-0.2607	-0.0165	-0.0096	-0.0131
β_n	2.2329	-1.0275	3.5623	-3.1828	6.2295	-7.2577

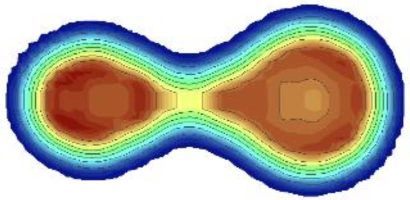
Comparison of scission configurations



- Symmetric and asymmetric fission valleys are consistent
- **Nearly linear relation between Z_F (A_F) and q_3**, but not β_3: Jumps and plateaus
- Not so reasonable in large (β_2, β_3).

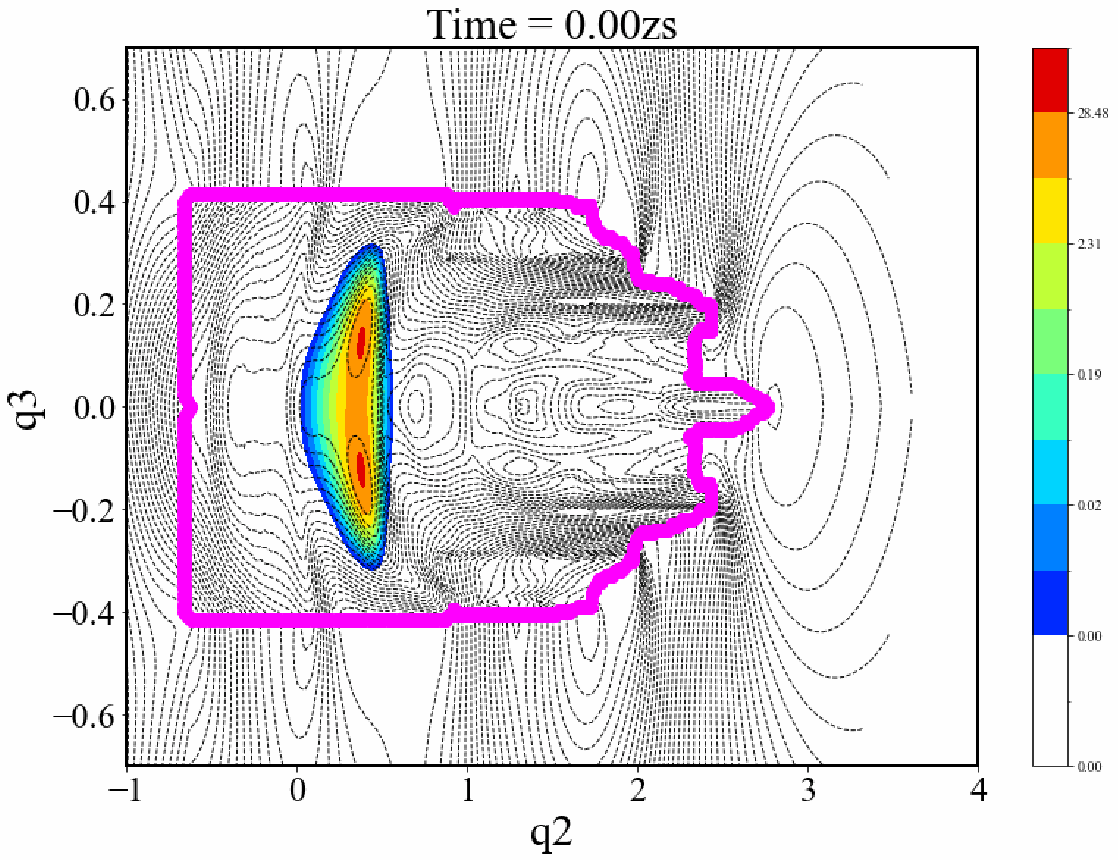


Spherical Harmonic

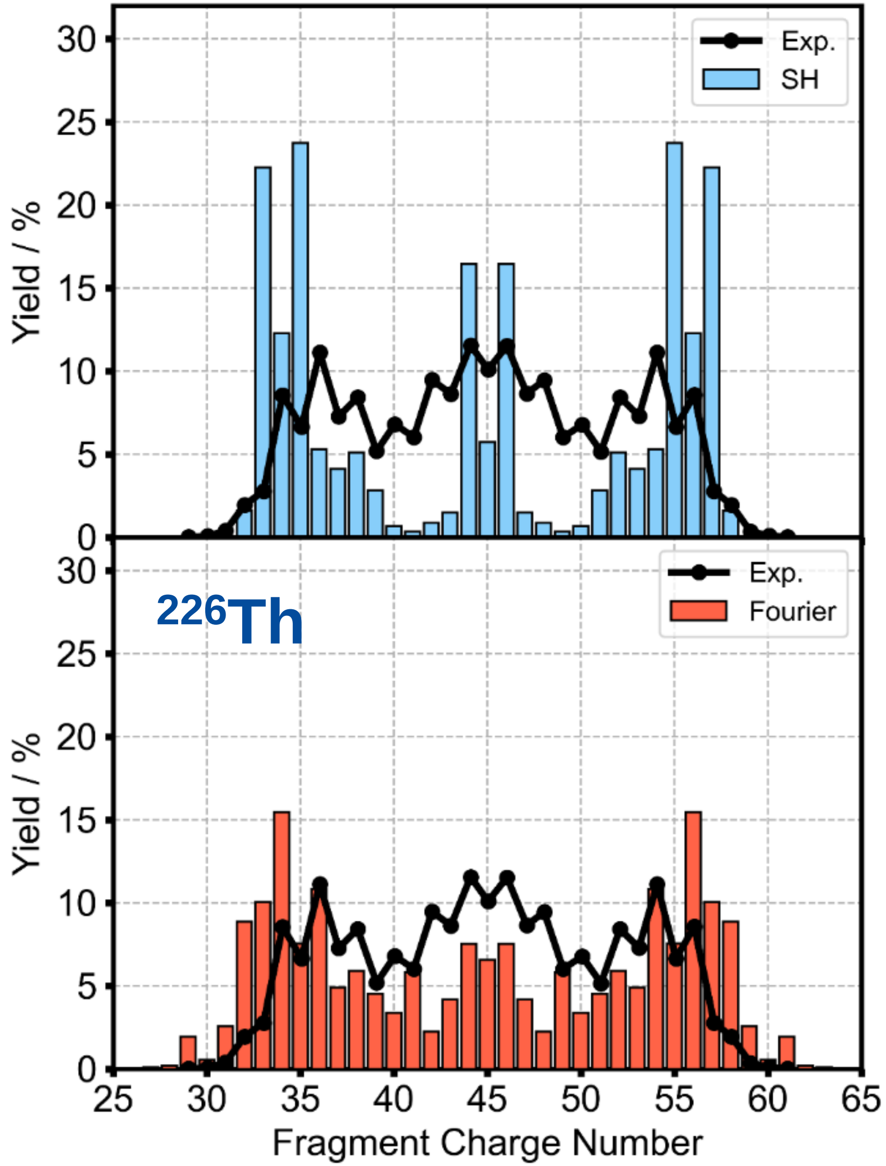


Fourier

Fission fragment charge distribution



K.-H. Schmidt, et al. Nucl. Phys. A665, 221 (2001)

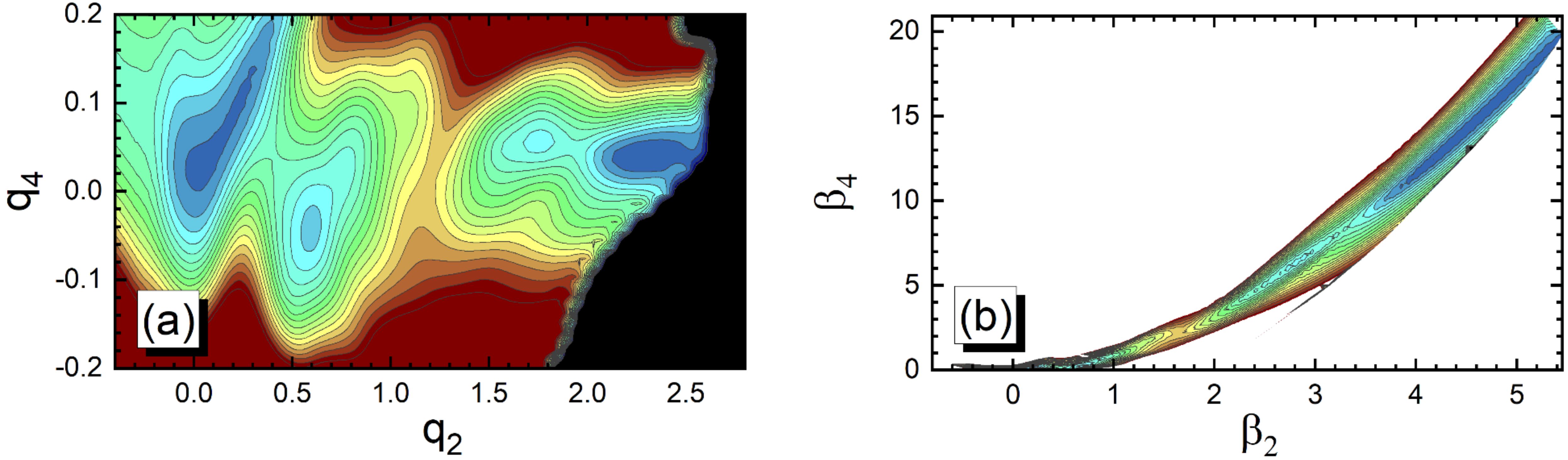


- **More fluctuations** in fragment charge distribution.
- The peak height and position that still need to be improved in further 3D calculation.

PESs in q_4 and β_4

PES in (q_2, q_4) plane with $q_3 = 0$

PES in (β_2, β_4) plane with $\beta_3 = 0$



- PES in (q_2, q_4) plane is smooth; Scission configurations are easy to obtain
- While for (β_2, β_4) plane, β_4 has strong correlation with β_2.

Li, Su, Chen & ZPLi, to be submitted

Summary and outlook

西南大學

- **Relativistic DFT based on TCHO basis**
  - Better accuracy and efficiency; possibility for post-scission
- **Based on RDFT-TCHO & TDGCM+GOA**
  - Asymmetric fission of ^{180}Hg: N=56 octupole shell gap
  - Sawtooth-like distribution of FAM; Strong correlation at φ_{LH}~30^{o}
  - Fourier shapes: fast convergence; better scission configurations …

Outlook: TDGCM based on 3D Fourier shapes; Y(A, Z) & P(S_L, S_H)

Finite temperature; dissipation …

Curriculum Vitae

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(3) September 2015 - July 2019: **Bachelor of Science in Physics**, Sichuan Normal University.

Thanks for your attention!

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M. S. Smith	*ORNL*
J. Zhao	*Pengcheng Lab.*
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