Fission barriers for r-process nuclei

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Outline

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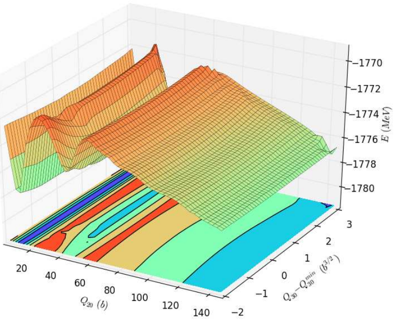
The fission process of heavy and superheavy nuclei

- Important for the r-process nucleosynthesis: fission cycling is a mechanism to obtain a robust r-process.
- Useful to study the influence of magic numbers in nuclear structure.
- Hypothetical island of stability?
- Nuclei far from stability: theoretical models required!

Fission within the Energy Density Functional approach

Two main ingredients:

- Potential Energy Surface:
  energy evolution from the ground state to the scission point.



- Collective inertias.

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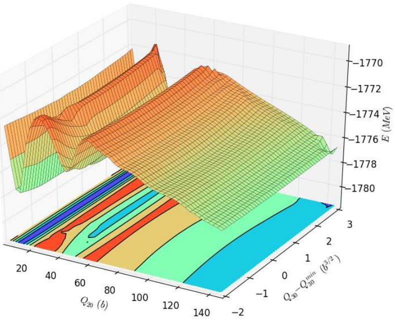

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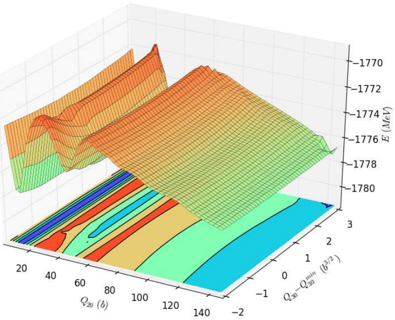


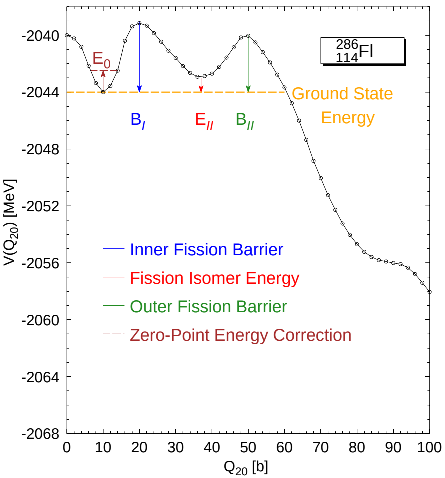
- Collective inertias.

  Hard to compute exactly!

  Different approximations (adiabatic, cranking, perturbative. . .).

Fission observables

- Parameters defining the potential energy surface:
  - inner and outer fission barrier heights,
  - isomer excitation energy.
- Fission lifetimes:
  - probability of tunneling under the fission barrier.



Theory of spontaneous fission lifetimes

Semiclassical approach given by the WKB formalism:

$$t_{\mathsf{sf}} = 2.86 \times 10^{-21}(1 + \exp(2S))\,.$$

Action along the (multidimensional) fission path s:

$$S = \int_a^b ds \sqrt{2 \times B(s)\left[E(s) - E_0\right]}\,.$$

- $B(s)$: Collective inertias
- $E(s)$: Potential energy
- E_0: Zero-Point Energy correction

Fission path given by:

- minimization of the action (dynamic approach),
- minimization of the energy (static approximation).

Outline

The BCPM energy-density functional

PHYSICAL REVIEW C **87**, 064305 (2013)

New Kohn-Sham density functional based on microscopic nuclear and neutron matter equations of state

M. Baldo*
Instituto Nazionale di Fisica Nucleare, Sezione di Catania, Via Santa Sofia 64, I-95123 Catania, Italy

- Density functional inspired in microscopic EoS,
- nuclear matter properties mapped onto finite nuclei models,
- good reproduction at masses (rms $\sim$ 1.6 MeV for even–even nuclei).

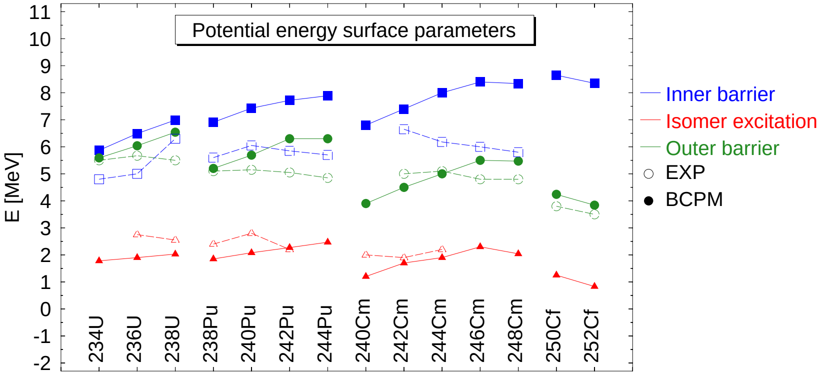
PHYSICAL REVIEW C **88**, 054325 (2013)

Fission properties of the Barcelona-Catania-Paris-Madrid energy density functional

Samuel A. Giuliani* and Luis M. Robledo†
Departamento de Física Teórica, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
(Received 26 August 2013; revised manuscript received 21 October 2013; published 27 November 2013)

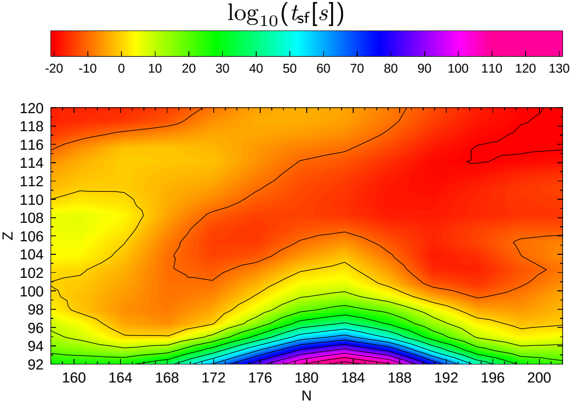
BCPM barrier heights and isomer energy

Exp: B. Sing et al., Nucl. Data Sheets **97**, 241 (2002); R. Capote et al., Nucl. Data Sheets **110**, 3107 (2009).



- Outer barrier and isomer energy values quite well reproduced for all nuclei.
- Inner barriers are reduced when triaxiality is allowed (Erler+(2012), Guzmán+(2014)).

The superheavy nuclear landscape: fission properties



- For $Z \leq 106$ peak of stability at $N = 184$ (predicted magic number!).
- Lightest nuclei: neutron-rich isotopes $\sim$ stable against spontaneous fission.
- High barriers around $N = 160 - Z = 104$.

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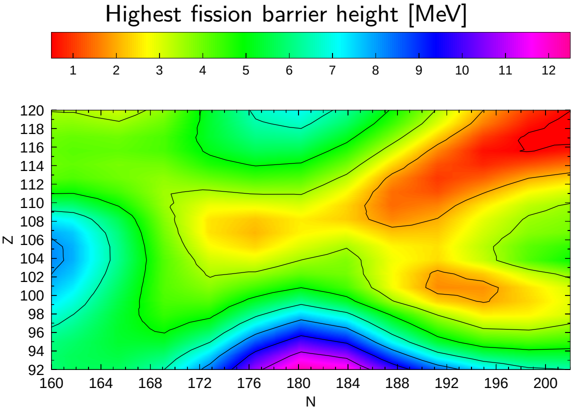

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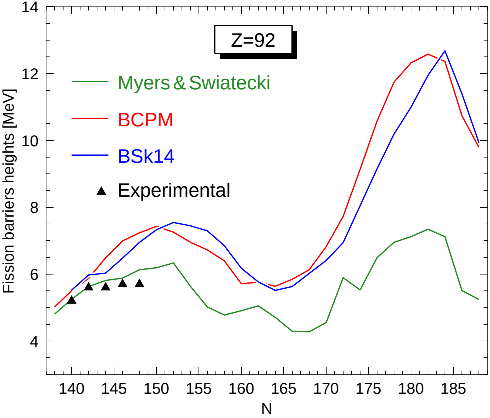
- Lightest nuclei: neutron-rich isotopes $\sim$ stable against spontaneous fission.
- High barriers around $N = 160 - Z = 104$.

Uranium fission barrier heights: theoretical predictions



Enhancement around $N = 184$ also predicted by other models!

Myers & Swiatecki: Myers et al., Phys. Rev. **C60**, 014606 (1999).

BSk14: Goriely et al., Phys. Rev. **C75**, 064312 (2007)

Outline

Pairing and spontaneous fission lifetimes

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- Fission path determined by minimizing $E(Q_{20})$.
- Q_{20} as collective degree of freedom.

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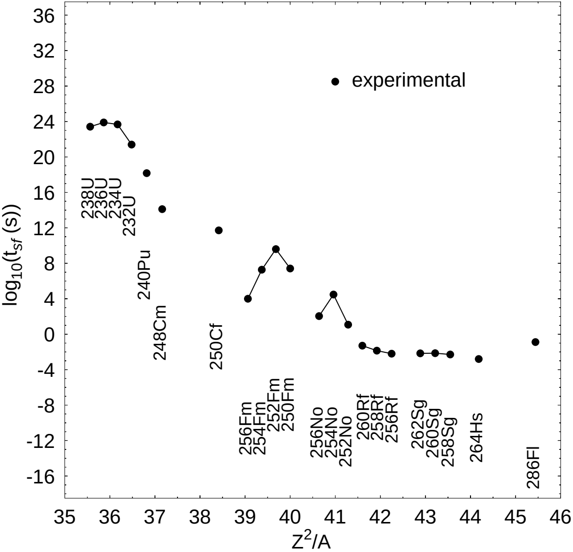
pairing correlations strengths: impact on t_{sf}?

η: multiplicative factor of the pairing gap field

Spontaneous fission lifetimes (BCPM results)

• Exp: Xiaojun Bao et al., Nucl. Phys. **A906**, 1–13 (2013).



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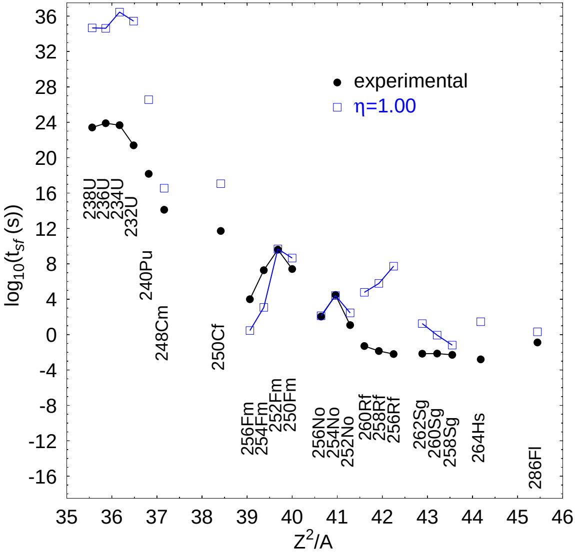

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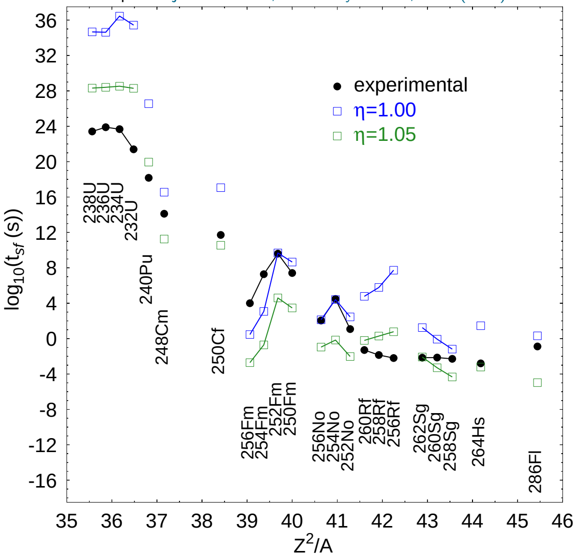

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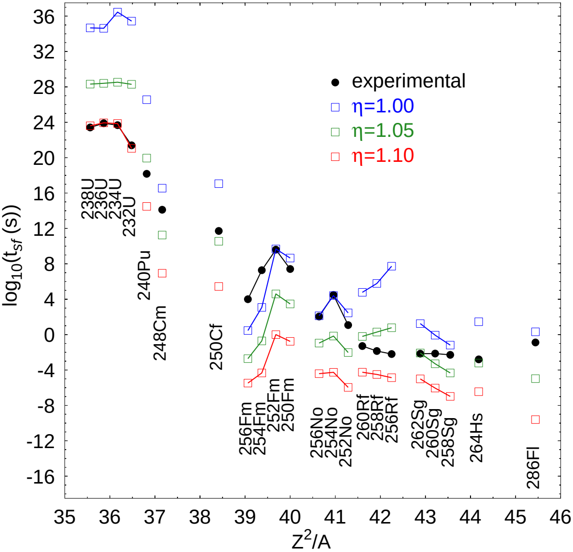

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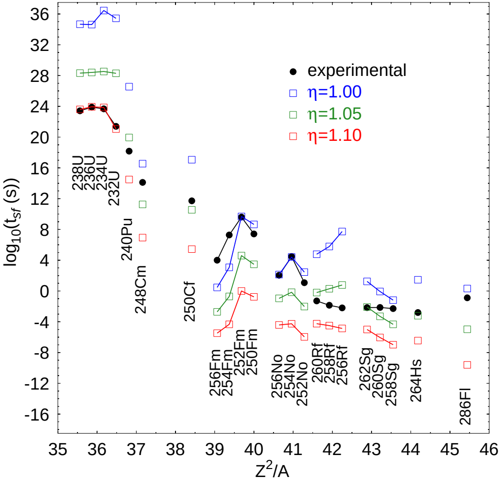
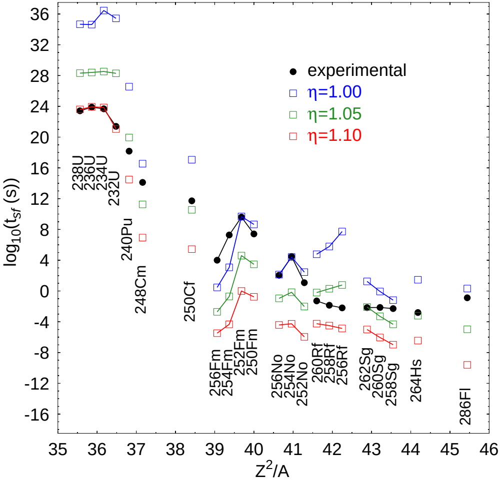


Increasing pairing strength η

smaller t_{SF} (by 12-13 OM).

- SAG and Robledo, Phys. Rev. **C88**, 054325 (2013).

Pairing and spontaneous fission lifetimes



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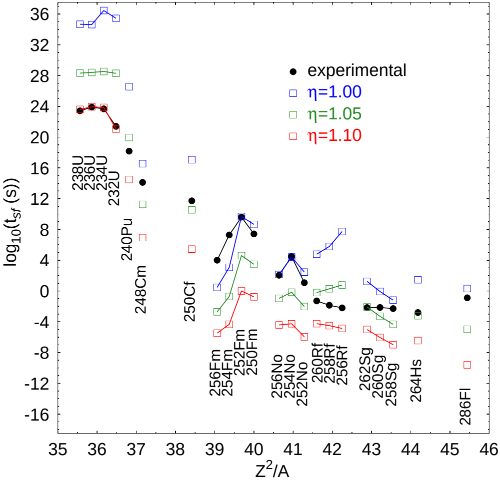

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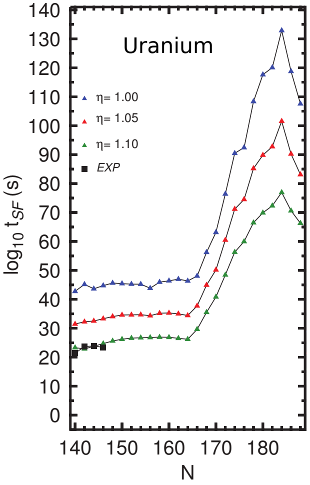

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Gogny

Same results obtained using the Gogny force.

- Guzmán and Robledo, Phys. Rev. **C89**, 054310 (2014).

Conclusions from pairing impact on t_{SF}

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   - Fission path determined by minimization of the energy (dynamic description)

Conclusions from pairing impact on t_{SF}

1. Go beyond the traditional (static) approach of minimization of the energy
   - Fission path determined by minimization of the energy (dynamic description)
2. Use a measure of pairing correlations as a collective degree of freedom.

The origins of the dynamic approach

- 1972 – "Funny Hills" paper (Brack et al.): spontaneous fission lifetimes computed using the least action principle,

$$S = \int_a^b ds \sqrt{2 \times B(s) \left[E(s) - E_0 \right]} \,.$$

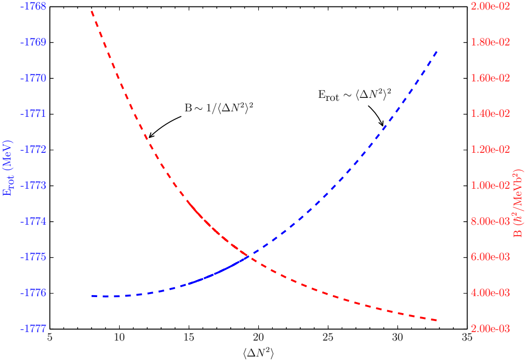
- 1974 – L.G. Moretto and R.P. Babinet: pairing gap Δ as degree of freedom of a simple fission model,

$$B \sim \frac{1}{\Delta^2}; \quad V(s) = V_0(s) + 2g(\Delta - \Delta_0)^2 \,.$$

- As a measurement of pairing correlations, the Δ parameter can be replaced by the particle number fluctuation $\Delta N^2 = N^2 - \langle N^2 \rangle$.

Minimizing the action: $B(\Delta N^2)$ vs $E(\Delta N^2)$ - ^{234}U

$$S = \int_a^b ds \sqrt{2 \times B(s)\left[E(s) - E_0\right]}$$



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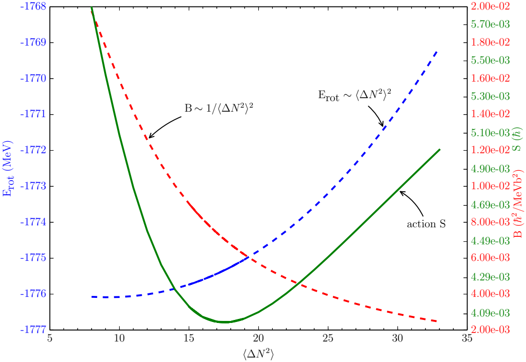

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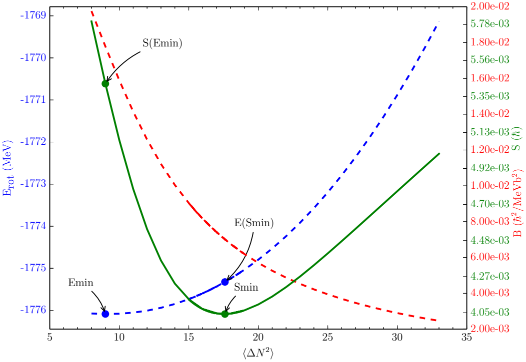

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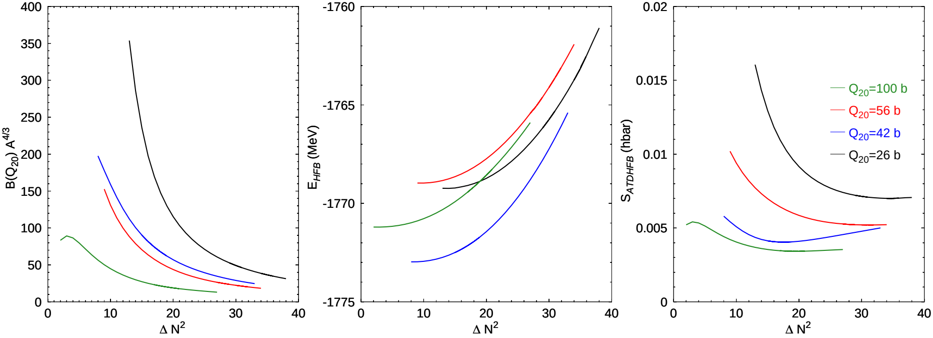
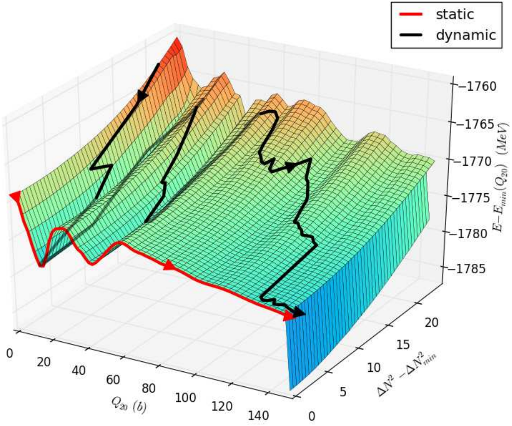


SAG, L. M. Robledo and R. Rodríguez-Guzmán, Phys. Rev. **C90**, 054311(2014)

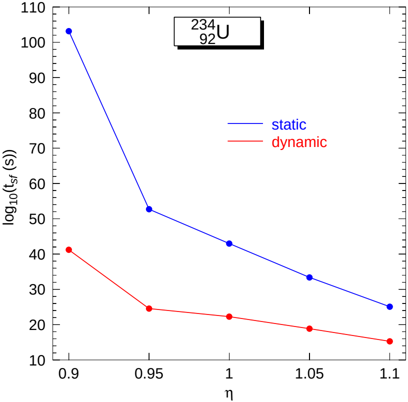
- S_{min} strongly differ from $S(E_{\text{min}})$ (selfconsistent value).

The least action path



- The least action path (black) strongly differ from the least energy one (red)!

dynamic *vs* static approach



- Large quenching of the spontaneous fission lifetimes.
- Results more robust against changes in the pairing strength η!

Outline

Conclusions

- EDF gives a good qualitative description of the fission process.
- But there are several uncertainties:
  - pairing strength, relevant degree of freedom and something else (collective inertias, quantal fluctuations, BMF effects. . .).
- The least action principle is a more robust approach: less sensitivity to pairing strengths (and collective inertia. . .).
- But we are still dealing with 3-4 OM of uncertainties.
- **Future work:**
  - Convert fission barriers into fission rates.
  - Computation of the fission fragments distribution.
  - Exact computation of the collective masses.
  - A theory beyond HFB is demanded.

Thank you

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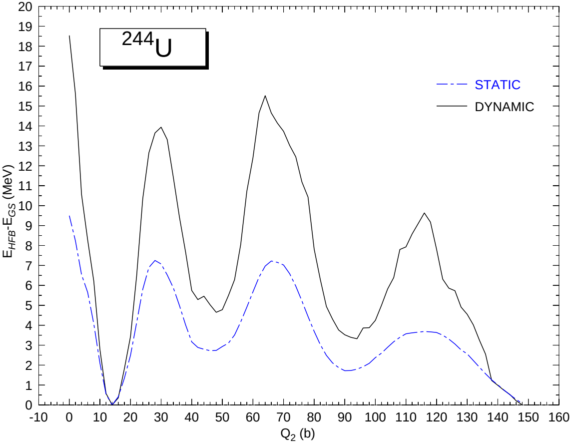
Fission barriers and E_0 - ^{244}U

$$S = \int_a^b ds \sqrt{2 \times B(s) \left[E(s) - E_0 \right]}$$



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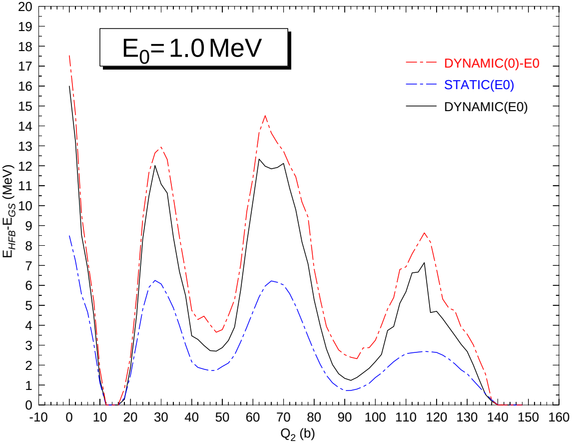

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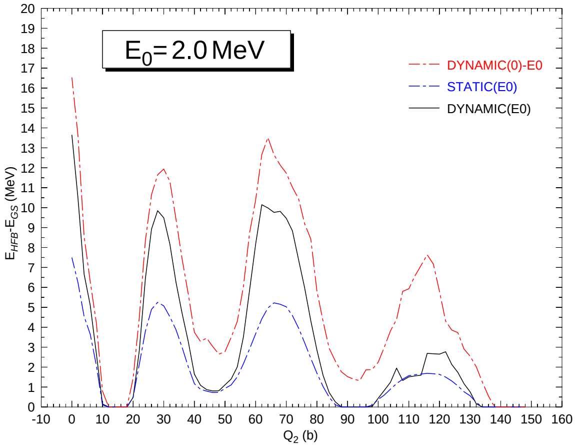

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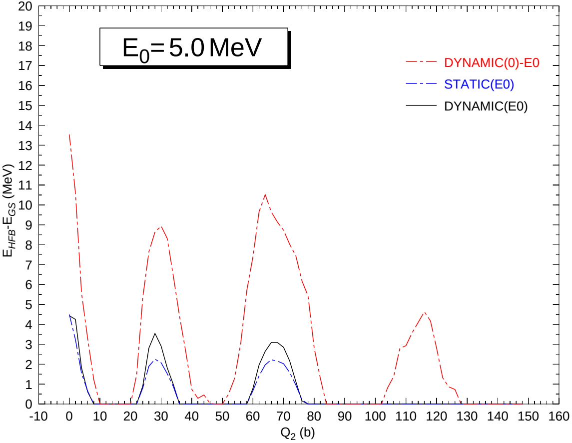


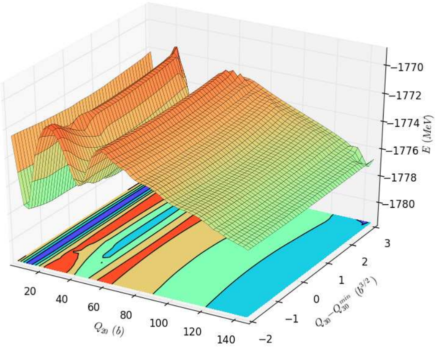
A microscopic approach: the Density Functional Theory

Two main ingredients:

- Evolution of the energy from the ground state to the scission point:
  - HFB theory with constrained field,
  - effective interactions (Skyrme, Gogny, RMF, others EDF. . .).
- Collective inertias associated to the fission path:
  - several theories (ATDHFB vs GCM),
  - different approximations (exact, cranking approximation, perturbative cranking approximation. . .)

Fission observables

- Spontaneous fission lifetimes:
  - computed using the WKB formula.
- Parameters defining the potential energy surface:
  - inner and outer fission barrier heights (model dependent),
  - isomer excitation energy.
- Fission fragments distribution:
  - phenomenological description



The energy-density functionals

PHYSICAL REVIEW C **88**, 054325 (2013)

Fission properties of the Barcelona-Catania-Paris-Madrid energy density functional

Samuel A. Giuliani* and Luis M. Robledo†
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(Received 26 August 2013; revised manuscript received 21 October 2013; published 27 November 2013)

- Density functional inspired in microscopic EoS,
- nuclear matter properties mapped onto finite nuclei models using LDA,
- good reproduction at masses (rms $\sim$ 1.6 MeV for even–even nuclei).

PHYSICAL REVIEW C **89**, 054310 (2014)

Microscopic description of fission in uranium isotopes with the Gogny energy density functional

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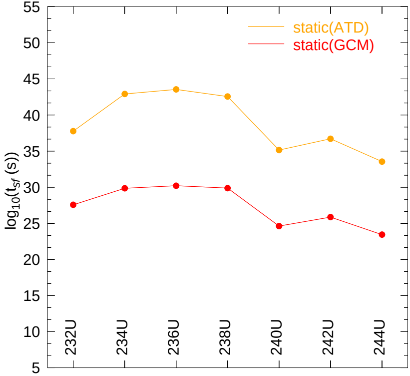
Department of Physics and Astronomy, Rice University, Houston, Texas 77005, USA
and Department of Chemistry, Rice University, Houston, Texas 77005, USA

L. M. Robledo†
Departamento de Física Teórica, Universidad Autónoma de Madrid, 28049 Madrid, Spain
(Received 27 December 2013; revised manuscript received 28 March 2014; published 8 May 2014)

- Finite range density dependent interaction,
- several fits including fission data (D1S) or even-even masses (D1M).

Theory of collective masses $B(s)$: GCM vs ATDHFB

$$t_{\mathsf{sf}} = t_0 \exp\left(\frac{2}{\hbar}\int_a^b ds\sqrt{2\cdot B(s)[V(s)-E_0]}\right)$$



- ATDHFB inertias roughly two times larger than GCM.

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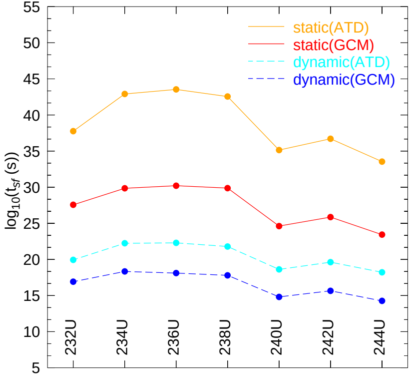
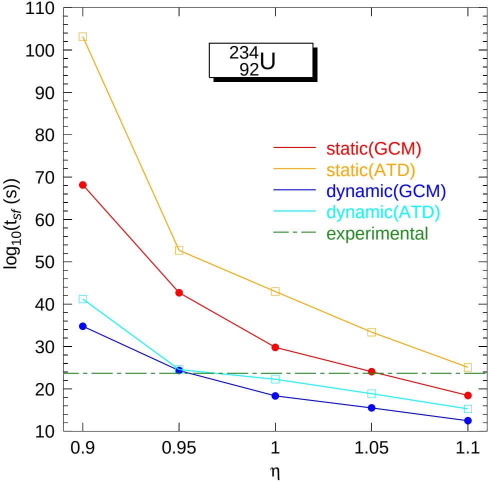


- ATDHFB inertias roughly two times larger than GCM.
- Results more robust against the collective inertias computations!

Summarizing. . .

dependence with η and B



Method	t_{sf} ATD (s)	t_{sf} GCM (s)
E_{min}	0.81×10^{43}	0.70×10^{30}
$S_{\mathrm{min}}(Q_{20}, Q_{30})$	0.44×10^{42}	0.64×10^{29}
$S_{\mathrm{min}}(Q_{20}, Q_{40})$	0.12×10^{43}	0.10×10^{29}
$S_{\mathrm{min}}(Q_{20}, \Delta N^2)$	0.18×10^{23}	0.21×10^{19}

The BCPM functional

The energy of a finite nucleus is given by

$$E = T_0 + E_{int}^{\infty} + E_{int}^{FR} + E^{s.o.} + E_C + E_{pair}$$

$$E_{int}^{\infty}[\rho_p, \rho_n] = \int d\vec{r} \Big[P_s(\rho)(1-\beta^2) + P_n(\rho)\beta^2 \Big] \rho$$

with $\rho(\vec{r}) = \rho_n(\vec{r}) + \rho_p(\vec{r})$ and $\beta(\vec{r}) = (\rho_n(\vec{r}) - \rho_p(\vec{r}))/\rho(\vec{r})$.

P_s and P_n are polynomial fits to reproduce microscopic EoS in nuclear matter.

- Phenomenological surface contribution

$$E_{int}^{FR}[\rho_n, \rho_p] = \frac{1}{2} \sum_{t,t'} \iint d\vec{r} d\vec{r'} \rho_t(\vec{r}) v_{t,t'}(\vec{r} - \vec{r'}) \rho_{t'}(\vec{r'})$$

with $v_{t,t'}(r) = V_{t,t'} \, e^{-r^2/r_{0\,tt}{}^2}$; $V_{n,n} = V_{p,p} = V_L = 2\tilde{b}_1/(\pi^{3/2} r_{0L}^3 \rho_0)$;
$V_{n,p} = V_{p,n} = V_U = (4a_1 - 2\tilde{b}_1)/(\pi^{3/2} r_{0U}^3 \rho_0)$.

M.Baldo et al. Phys. Lett. B663 (2008) 390; Phys. Rev. C87 064305 (2013)

Remaining contributions to the EDF

- Coulomb

  Direct $E_C^H = (1/2) \iint d\vec{r} d\vec{r'} \rho_p(\vec{r}) |\vec{r} - \vec{r'}|^{-1} \rho_p(\vec{r'})$

  Exchange: $E_C^{ex} = -(3/4)(3/\pi)^{1/3} \int d\vec{r} \rho_p(\vec{r})^{4/3}$
- Spin-Orbit

$$\hat{v}_{ij}^{so} = i W_{LS} (\vec{\sigma}_i + \vec{\sigma}_j) \cdot [\vec{k}' \times \delta(\vec{r}_i - \vec{r}_j) \vec{k}]$$

Free parameters

W_{LS} and r_{0L}, r_{0U}

- Pairing Correlations (E. Garrido et al. Phys. Rev. C **60**, 064312 (1999))

  Zero-range interaction,

$$v^{pp}(\rho(\vec{r})) = \eta \times \frac{v_0}{2} \left[1 - \gamma \left(\frac{\rho(\vec{r})}{\rho_0} \right)^{\alpha} \right], \qquad \rho_0 = \frac{2}{3\pi^2} k_F^3 \,.$$

  $\eta \equiv$ multiplicative parameter setting the pairing strength. . .