Physics

The Fission Process (II)

EBSS 2014 Summer School

W. Younes

Physical and Life Sciences

Lawrence Livermore National Laboratory

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Fission dynamics: the Time-Dependent Hartree-Fock method

- In general: $|\Psi(t)\rangle = \exp(-iHt/\hbar)\,|\Psi(0)\rangle$
  - For H = full many-body Hamiltonian, this is too difficult!
- Time-dependent Hartree-Fock (Bogoliubov)
  - Start with Slater determinant, assume it stays a Slater determinant

$$\hbar i \frac{\partial \rho}{\partial t} = \left[h(\rho), \rho \right]$$

  - The good:
    - introduces internal excitations through particle collisions
    - no need to choose collective coordinates a priori, the system finds its path on the energy surface
  - The bad:
    - Classical behavior (system follows a single trajectory)
    - Can't tunnel (due to conservation of energy)
    - Spurious final state interaction

For a full discussion, see Ring & Schuck chapter 12

Examples of fission calculations using TDHF

- J.W. Negele et al., Phys. Rev. 17, 1098 (1978)
  - Calculated ^{236}U induced fission times, compared with different dissipations/viscosities. Found fission times of $3\text{-}4\times10^{-21}$ s
- K. Dietrich and J. Nemeth, Z. Phys. A 300, 183 (1981)
  - Studied fission of slabs of nuclear matter
- J. Okolowicz, et al., J. Phys. G 9, 1385 (1983)
  - Compared calculations with one- or two-center Slater determinants
- A. S. Umar et al., J. Phys. G 37, 064037 (2010)
  - TDHF with constrained density, applied to the study of fission following heavy-ion collisions (e.g., ^{100}Zr + ^{140}Xe)

Fission dynamics: the time-dependent GCM

Replace the GCM ansatz with: $\left|\Psi(t)\right\rangle = \int dq\, f(q,t)\left|\Phi(q)\right\rangle$

Variational principle + 2nd order expansion in non-locality

$$H_{\text{coll}}\, g(q,t) = \hbar i \frac{\partial}{\partial t} g(q,t)$$

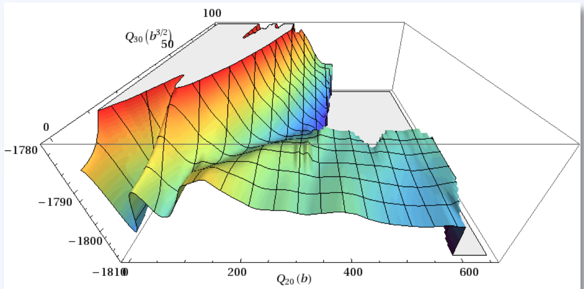
$$H_{\text{coll}} = -\frac{1}{2}\frac{\partial}{\partial q} B(q) \frac{\partial}{\partial q} + \left\langle \Phi(q) \middle| H \middle| \Phi(q) \right\rangle - \varepsilon_0(q)$$

Same collective Hamiltonian as in static GCM

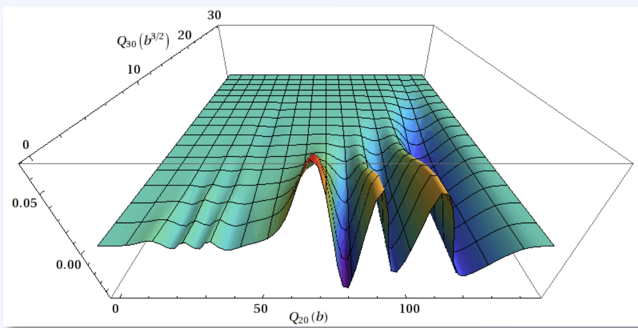
- To obtain microscopic, time-dependent picture of fission:
  - Calculate potential energy surface, inertia tensor, and initial state
  - Solve time-dependent collective Schrodinger equation
- See: J.-F. Berger et al., Comp. Phys. Comm. 63, 365 (1991); H. Goutte et al., Phys. Rev. C 71, 024316 (2005)

Application of the GCM: fission dynamics for ^{240}Pu

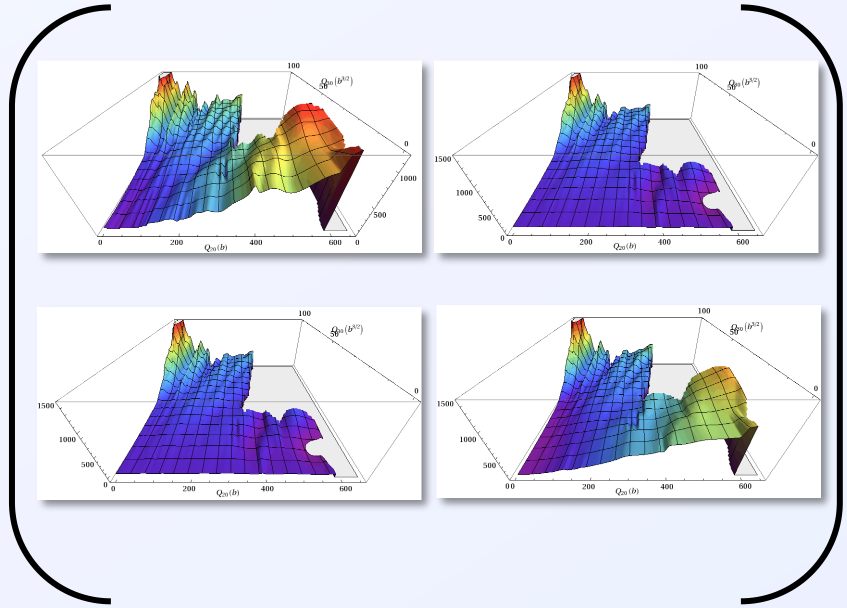
$V(Q_{20}, Q_{30}) =$



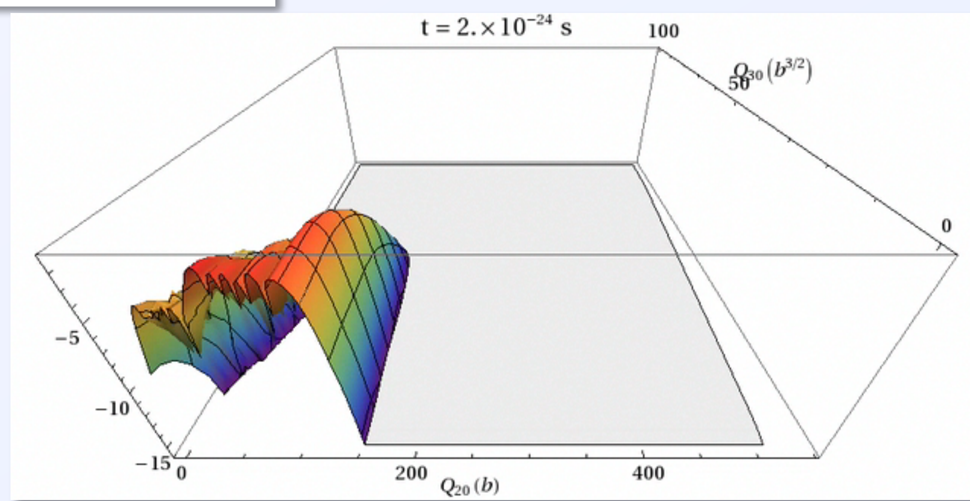
$g(t=0) =$



$B =$



$\log|g(t)|^2$



Coupling between intrinsic and collective excitations in fission

- **Develop GCM on a basis that includes intrinsic excitations**

$$\left|\Psi\right\rangle = \int dq\, f_0(q) \underbrace{\left|\Phi_0(q)\right\rangle}_{\text{HFB minima}} + \sum_{i\neq 0} \int dq\, f_i(q) \underbrace{\left|\Phi_i(q)\right\rangle}_{\text{excitations}}$$

- **Leads to generalized, non-adiabatic, Hill-Wheeler equation**
- **Can be reduced to Schrodinger-like equation**
  - **No need for extraneous dissipation mechanism: coupling between HFB minima and excited states is treated explicitly**
- **This promising approach is in development**
  - **See Bernard et al., Phys. Rev. C 84, 044308 (2011)**

Recap: the microscopic approach so far

Effective nucleon interaction (parameters)

Single-particle Hamiltonian

HFB

Constraints

$\Phi(q)$

$\Phi(q)$

$\Phi(q)$

⋮

GCM

2nd order in non-locality

Collective Hamiltonian

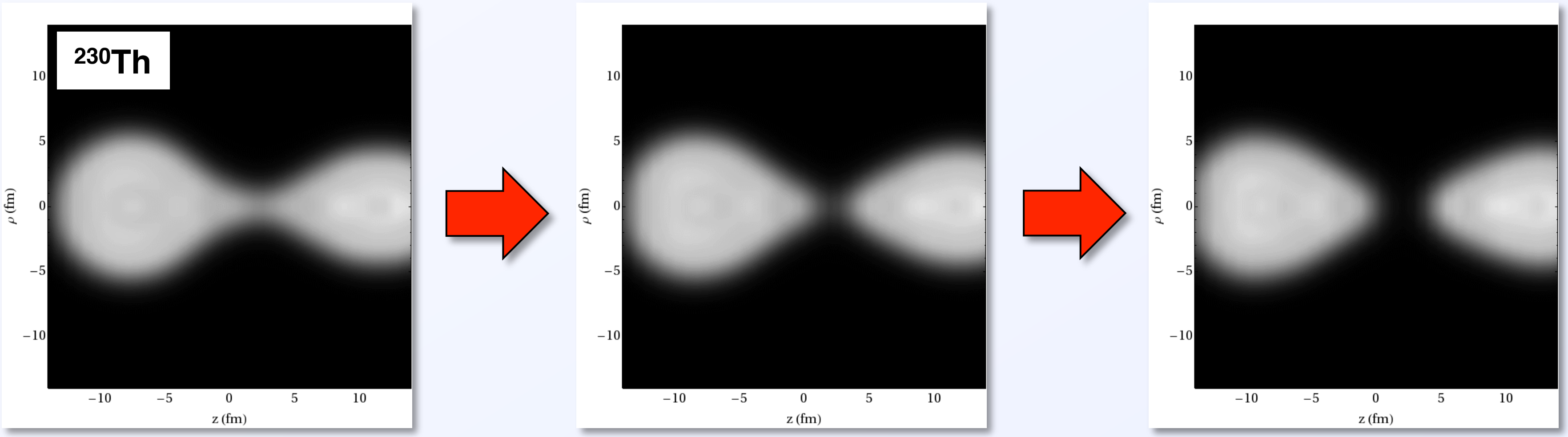
TDGCM

Time-evolution of the nucleus Toward…

See, e.g.,
J.-F. Berger et al., Nucl. Phys. A502, 85 (1989)
H. Goutte et al., Phys. Rev. C 71, 024316 (2005)

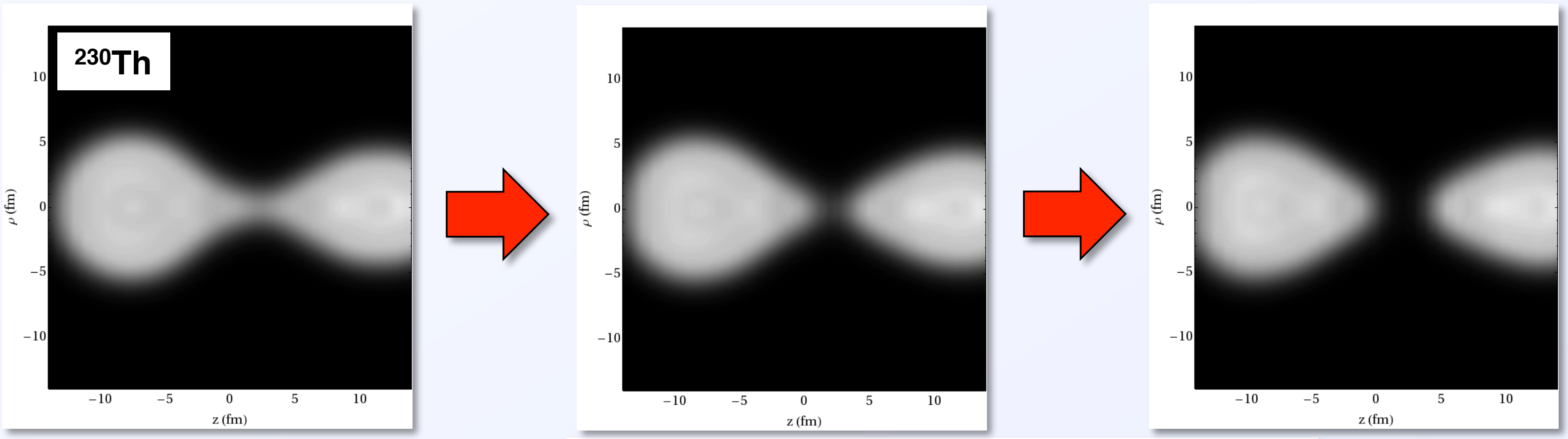
We're missing a crucial ingredient: scission

The nucleus near scission



Microscopic calculation of the final stages of fission

The nucleus near scission

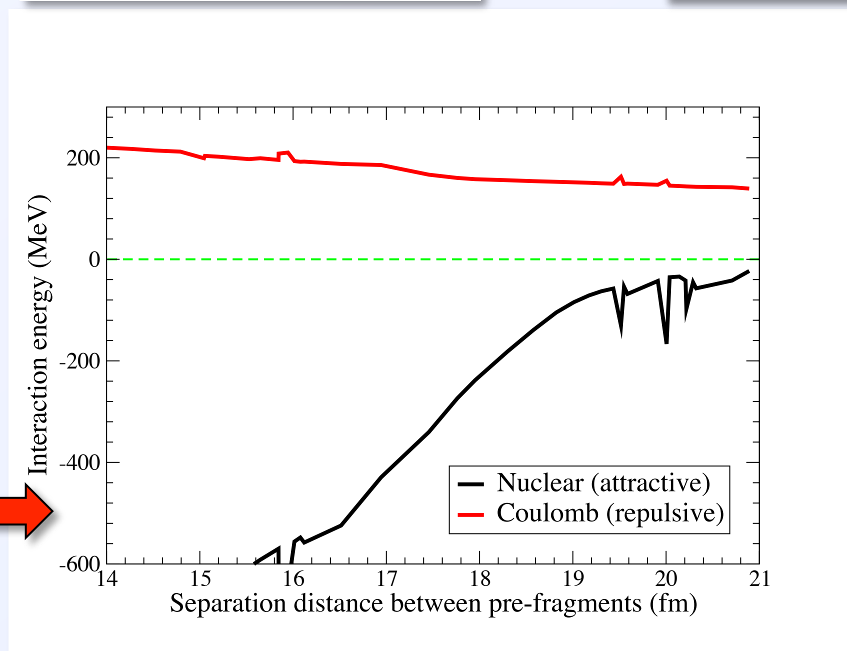


but calculate the **nuclear interaction energy** between fragments in last panel:

E_{int} = -68.3 MeV

Not negligible!

In fact, look as a function of fragment separation:

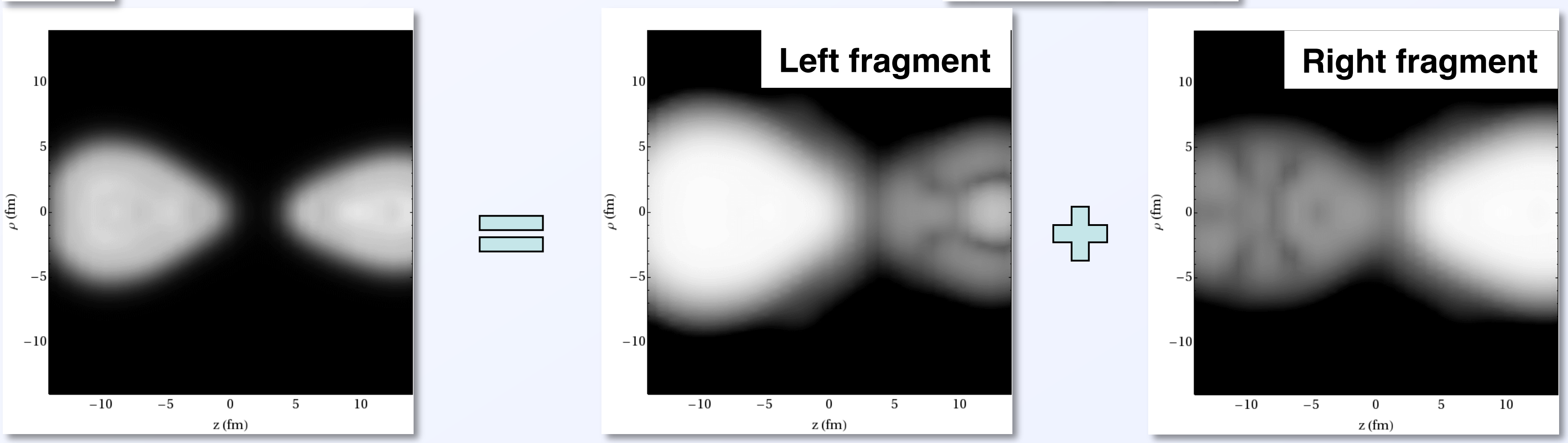


So where does scission occur?

The nucleus near scission

^{230}Th

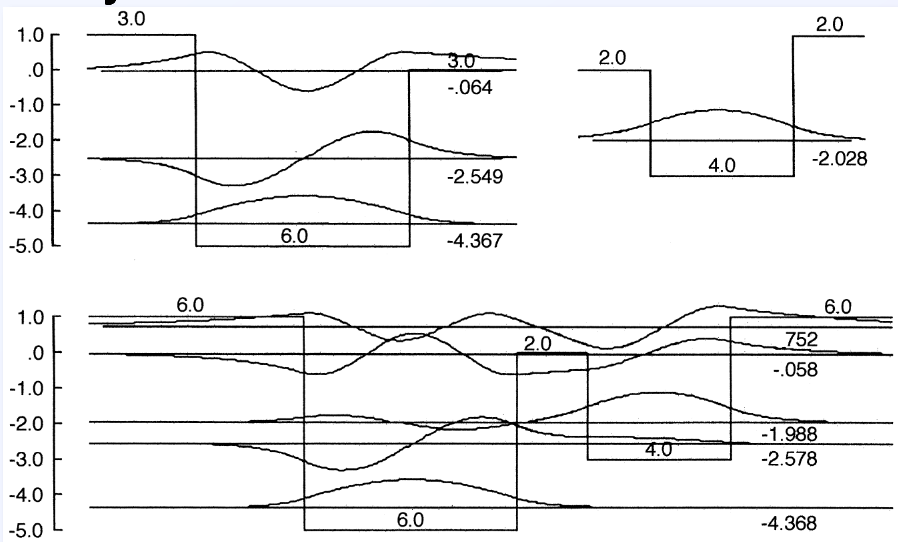
(Note: log scale)



- The nucleon wave functions are <u>delocalized</u>, i.e., the fragments have tails!
- Tails are small but venture deep into complementary fragment!
  - Keep in mind: total <u>nuclear</u> energy of ^{230}Th in G.S. ~ -6.6 GeV
  - Each particle in tails contributes ~ -50 MeV to nuclear interaction between fragments
- We are dealing here with the non-local nature of quantum mechanics!

The quantum localization problem

- In QM, the double-well potential gives rise to delocalized orbitals (see, e.g., R. Gilmore, "Elementary Quantum Mechanics in One Dimension", JHU press (2004)):



- This is not a numerical issue, a basis problem, or a problem that is unique to nuclear fission: it is a direct consequence of the non-local nature of QM
- We encounter the same situation with fission, and the calculation of the interaction between fragments is based on these orbitals

How do we recognize pre-fragments progressively, and extract their properties near scission using criteria based on their interaction energy?

The concept of Localized Molecular Orbitals (LMOs)

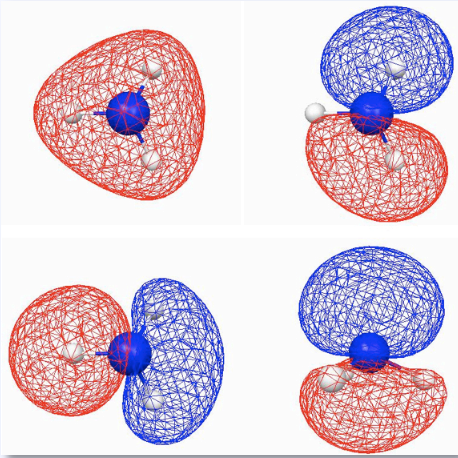
Sir John Lennard-Jones, Proc. Roy. Soc. A 198, 14 (1949):

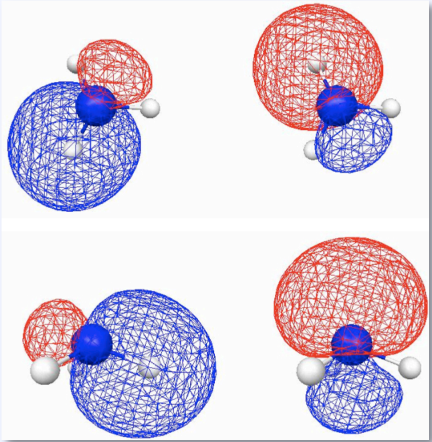
The equations (2·01) were obtained from a determinantal wave function of the form

$$\Phi = \mathrm{Det}\{\psi_1(1)\,\alpha(1)\,\psi_1(2)\,\beta(2)\ldots\psi_p(2p-1)\,\alpha(2p-1)\,\psi_p(2p)\,\beta(2p) \times \psi_{p+1}(2p+1)\,\alpha(2p+1)\ldots\psi_{p+q}(2p+q)\,\alpha(2p+q)\}, \quad (3{\cdot}01)$$

and the properties of the system will not be altered by any transformation which leaves this wave function unchanged. Thus any orthonorm transformation of the functions ψ_1 to ψ_n, which constitute its elements, will not change Φ. It is unchanged

Bogoliubov vacuum is invariant under unitary transformations of destruction operators



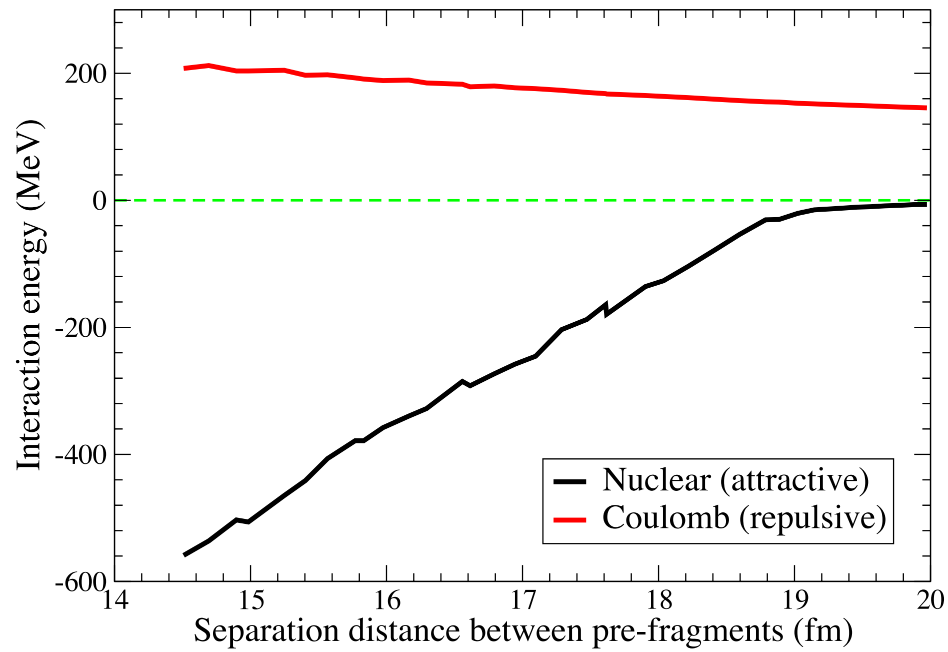


NH_3: linear combinations of canonical molecular orbitals chosen to minimize repulsion between the 4 valence electron pairs (Jan H. Jensen, "Molecular Modeling Basics" CRC Press (2010).

For fission: choose representation that is appropriate to scission!

The nucleus near scission: quantum localization

- So find a unitary transformation that reduces the tails
- Now we can describe fission up to scission, and beyond



Younes & Gogny, Phys. Rev. Lett. 107, 132501 (2011)

We have a quantum-mechanical definition of scission!

The quantum-mechanical definition of scission

1) Coulomb force >> nuclear attraction between pre-frags (e.g., × 30)
2) Exchange interaction is small (e.g., < 1 MeV)
   - ⇒ To good approx, can neglect antisymmetry between fragments
   - ⇒ $|\tilde{0}\rangle \approx |\tilde{0}\rangle_1 \times |\tilde{0}\rangle_2$ for all quantities of interest (energies, moments,…)
3) Can excite local set of 2-qp states on each fragment

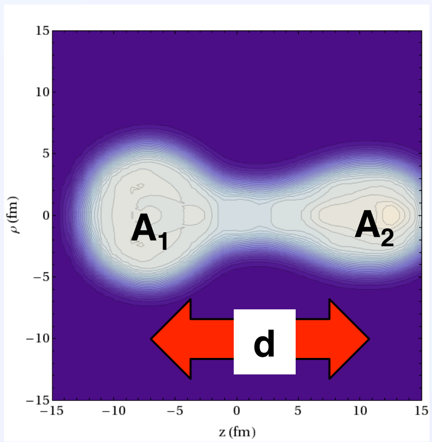
Fragments are separate entities, with their own excitations, and interacting only through a repulsive force acting only on their respective centers of mass

We need better collective coordinates near scission

- We want scission point for each mass division
- Traditionally: Q_{30} used to explore different mass divisions
- In practice: there isn't a one-to-one relation between Q_{30} and A
- In the conclusion to our PRL, we stressed the importance of <u>local</u> constraints (constraints on the individual pre-fragments)
- So, instead of Q_{20} and Q_{30}, we work with:

$$d \equiv z_2 - z_1$$

$$\xi \equiv \frac{A_2 - A_1}{A}$$



with

$$A_1 = \int_0^{2\pi} d\varphi \int_0^{\infty} r\,dr \int_{-\infty}^{z_N} dz\,\rho(r,\varphi,z)$$

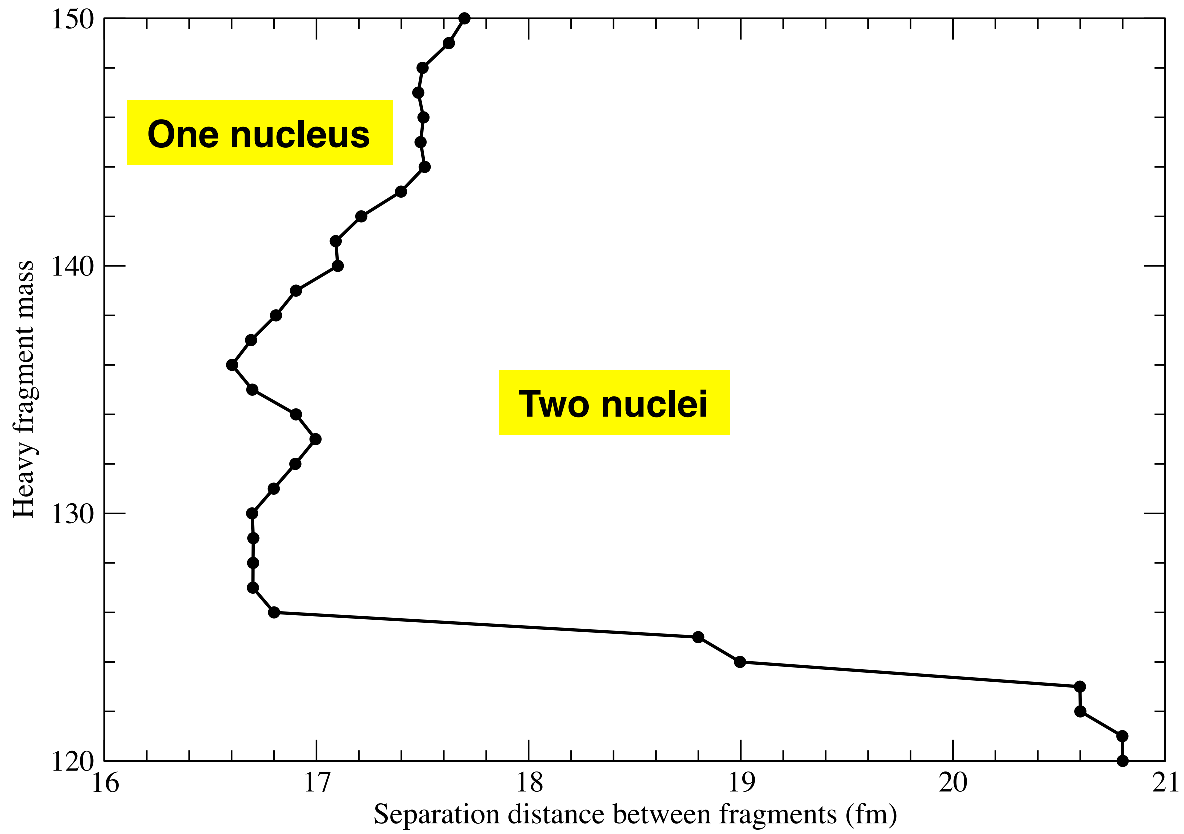
$$A_2 = \int_0^{2\pi} d\varphi \int_0^{\infty} r\,dr \int_{z_N}^{\infty} dz\,\rho(r,\varphi,z)$$

$$z_1 = \frac{1}{A_1}\int_0^{2\pi} d\varphi \int_0^{\infty} r\,dr \int_{-\infty}^{z_N} dz\,\rho(r,\varphi,z)\,z$$

$$z_2 = \frac{1}{A_2}\int_0^{2\pi} d\varphi \int_0^{\infty} r\,dr \int_{z_N}^{\infty} dz\,\rho(r,\varphi,z)\,z$$

Although constraints use semiclassical definitions of *d* and ξ, subsequent analysis of FF scission points uses quantum localization

The scission line in the new coordinates



How do we get the probability of populating the scission points?

- Answer: by calculating the dynamic evolution to scission
- The idea: derive collective Hamiltonian that governs that evolution
- Derivation inspired by Gaussian Overlap Approx to Hill-Wheeler eqs

$$H_{\text{coll}} = \underbrace{-\frac{1}{2}\sum_{x,y=d,\xi}\frac{\partial}{\partial x}B_{xy}(d,\xi)\frac{\partial}{\partial y}}_{\text{Kinetic energy}} + \underbrace{V(d,\xi)}_{\text{Potential energy}}$$

- In our approach we have an interior region (collective H for 1 nucleus) and an exterior region (Hamiltonian for 2 separate fragments), separated by scission boundary
- Solution in internal region gives flux across scission boundary (interpreted as rate) ⇒ mass distribution
- For each initial state at a given excitation energy, we calculate the propagation of the wave function and obtain the flux along the scission boundary, and therefore the mass distribution

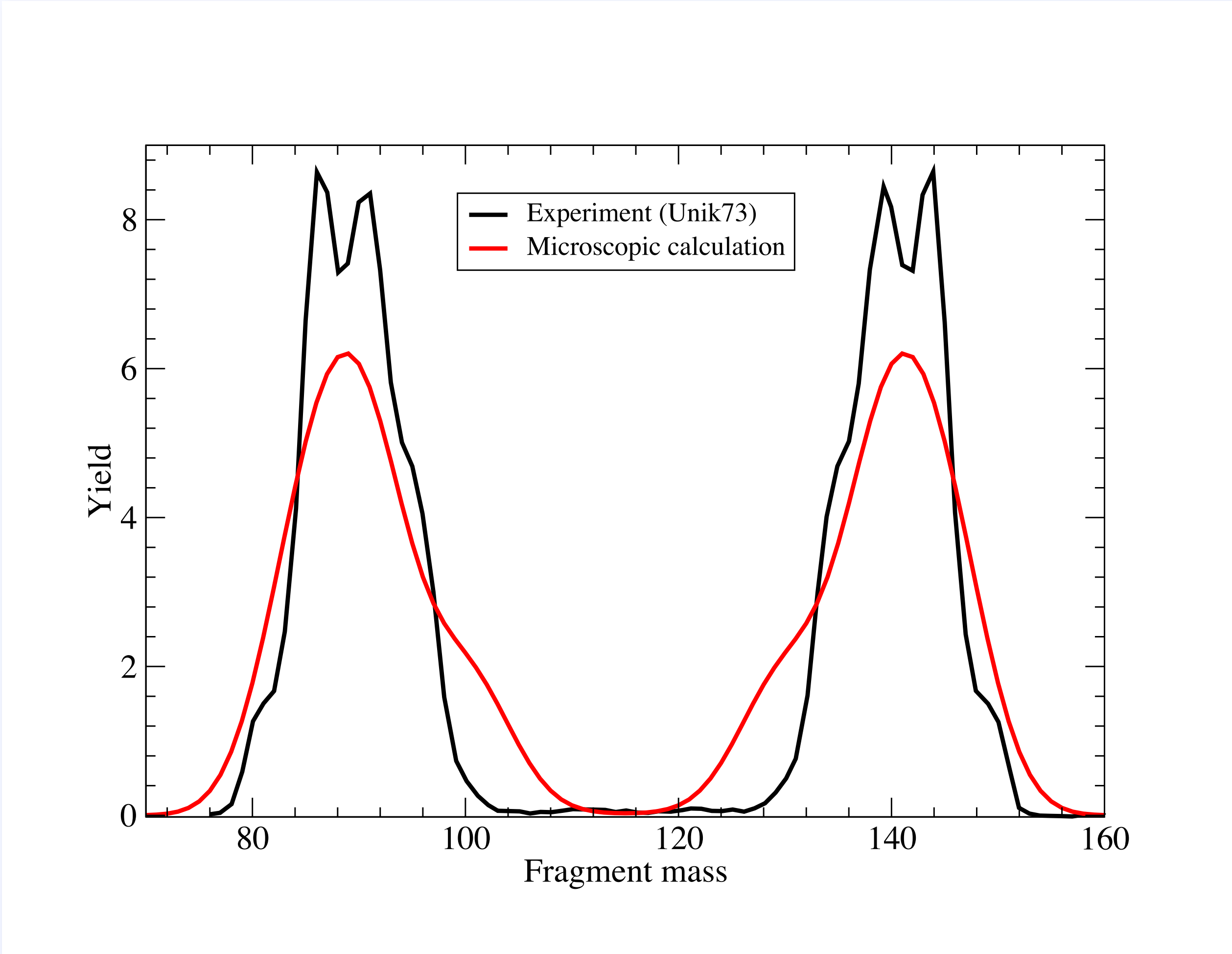
How do we connect interior and exterior regions?

- Up to scission: adiabatic HFB calcs, at scission the fragments are "frozen" in their configurations (molecular model: W. Nörenberg, 1969)
- We make the assumption that beyond scission, the fragments propagate according to a Hamiltonian that depends only on their separation

$$H_{\text{coll}} = \frac{\vec{p}_d^{\,2}}{2\mu m} + V(d) + E_1 + E_2 + \varepsilon_0$$

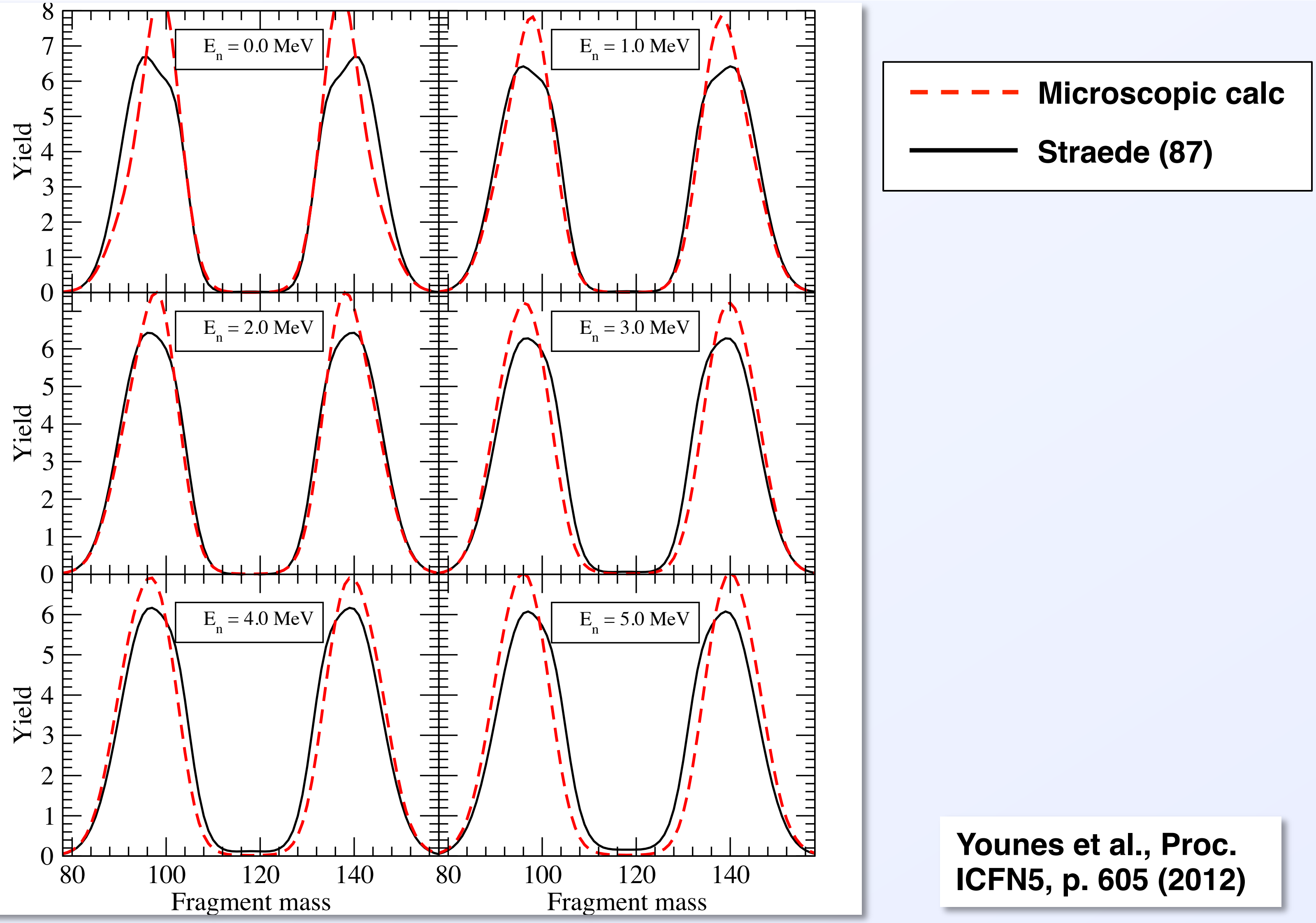
  - Where V(d) is the interaction between FF (i.e., Coulomb), E_1 & E_2 are the (constant) internal energies of the fragments and ε_0 is a zero-point energy that gives the center-of-mass correction
- At scission, we can calculate $V(d_{sc})$ from static HFB, we therefore need $p^2/2\mu m$ at scission (also known as the pre-scission kinetic energy) to calculate the TKE of the FF

Pre-neutron fission yields for ^{229}Th(n_{th},f)



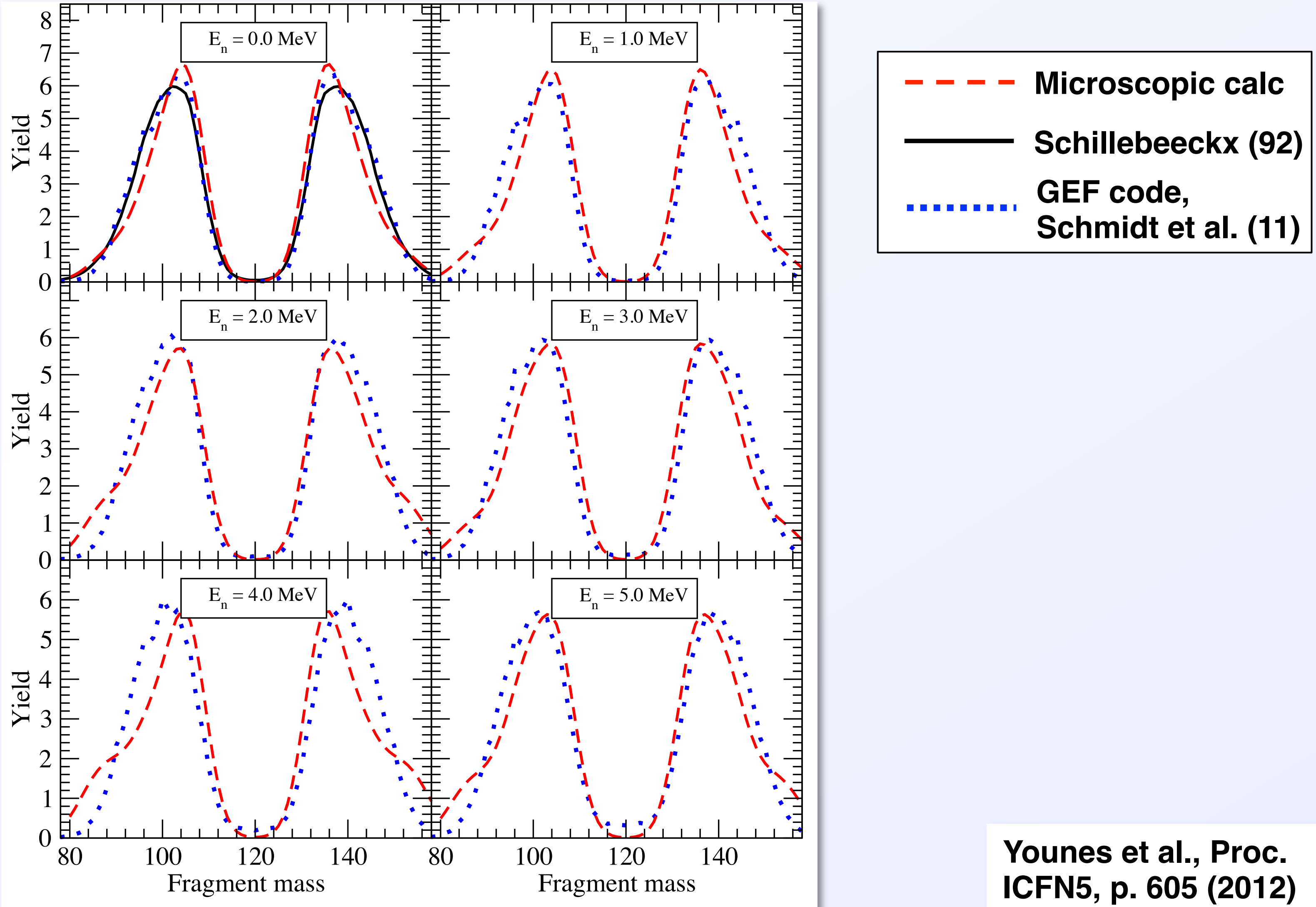
Starting from protons, neutrons, and effective interaction: Results consistent with experiment!

Fission dynamics: $^{235}U(n,f)$ mass distributions for E_n = 0-5 MeV



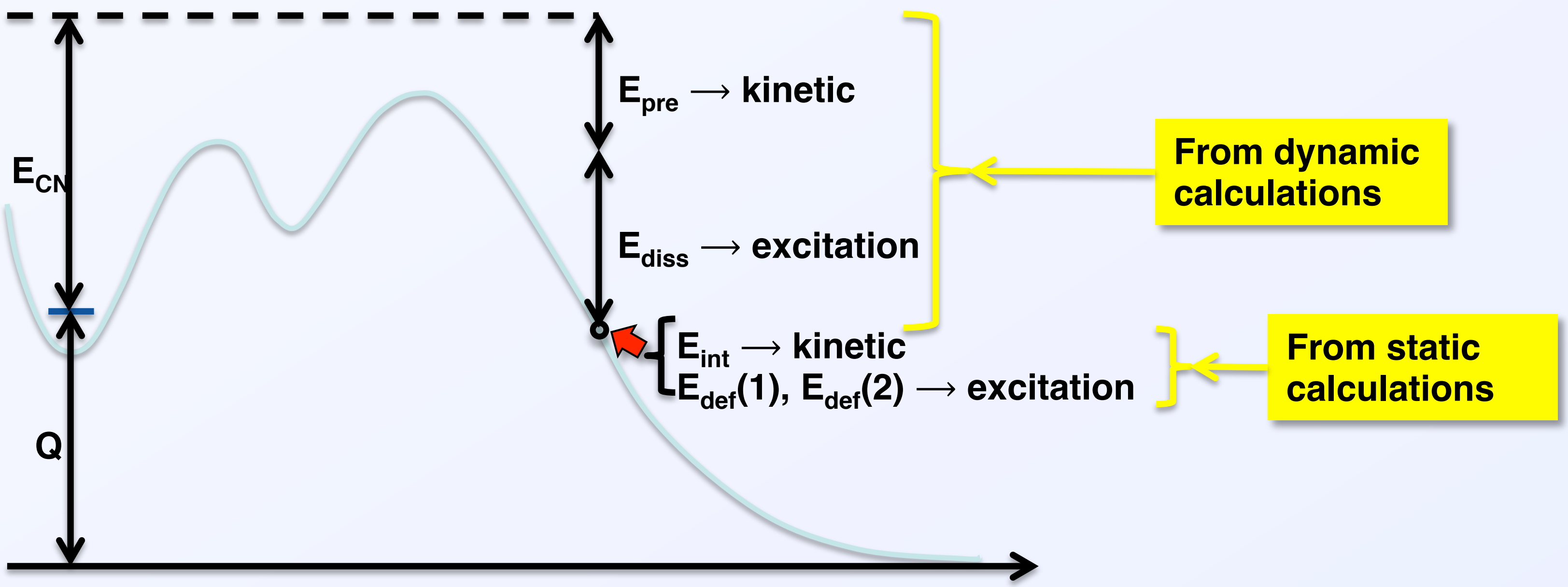
Younes et al., Proc. ICFN5, p. 605 (2012)

Fission dynamics: ^{239}Pu(n,f) mass distributions for E_n = 0-5 MeV



Younes et al., Proc. ICFN5, p. 605 (2012)

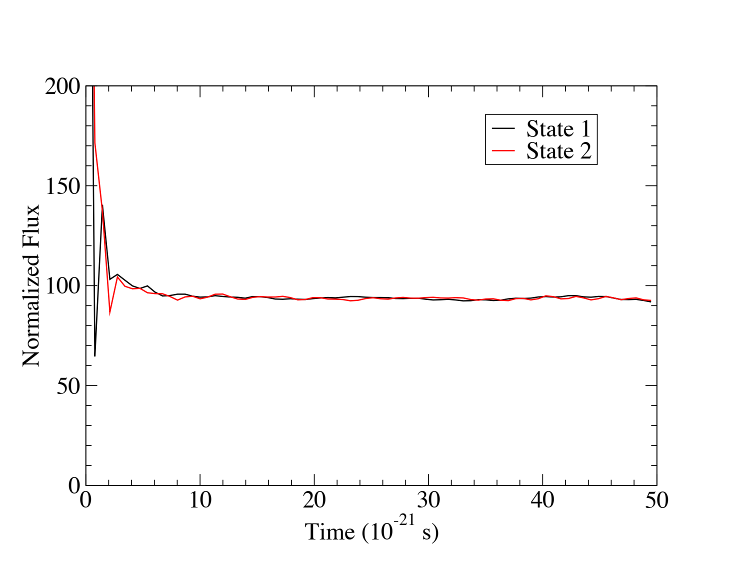
Calculating fragment energies



- Static contribution, After quantum localization of pre-fragments:
  - Identify scission configurations:
  - Integrate energy density for each fragment separately, allow each to relax to its minimum energy, difference gives excitation energy
  - Coulomb energy gives kinetic energy
- Dynamic contribution (pre-scission energy)

Estimate of the pre-scission kinetic energy

- Identify fission direction with direction of maximum flux at a scission point (near scission coincides with change in separation *d* between pre-FF)
- Calculate flux in that direction, normalized by squared amplitude of the wave function at this point
  - We observe that this normalized flux is ≈ constant in time



- This suggests a solution at scission that is a product of a local plane wave in the fission direction, and another function in the transverse direction (which cancels out in the normalized flux)

Estimate of the pre-scission kinetic energy

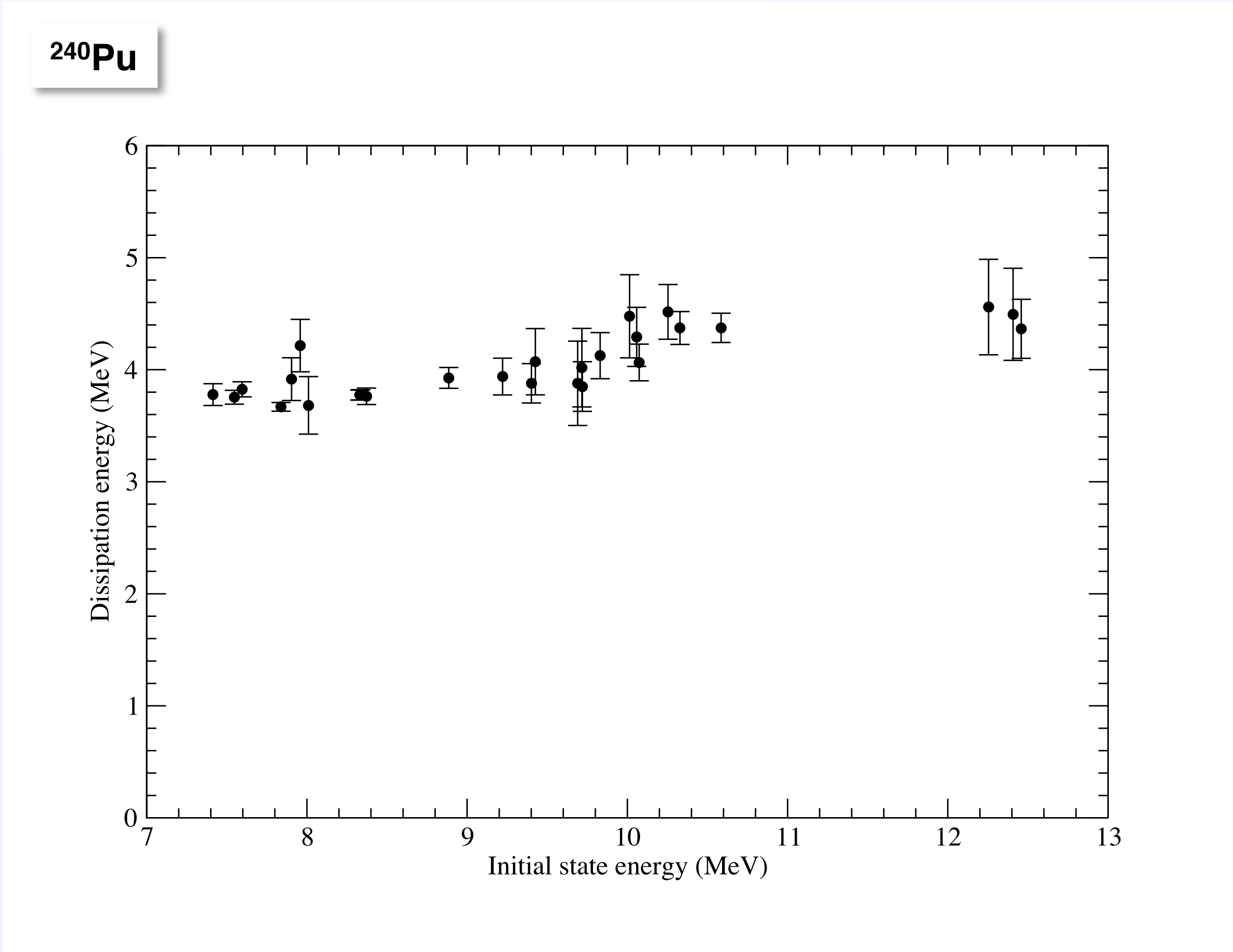
- **We make a WKB approximation in the fission direction to relate the normalized flux to the energy E_F of the wave in that direction**

  $$\phi / |g|^2 = \tfrac{1}{\hbar}\sqrt{2B_F E_F}$$ with B_F = inertia in fission direction

- We deduce E_F, which is smaller than what we would get in a 1D model without transverse motion ($E_F < E_{tot} - V_{sc}$)
  - We find E_F ~ 8 MeV out of 15 MeV available from saddle to scission
- We interpret E_F as the pre-scission kinetic energy
- The difference $E_{tot} - E_F$ is lost to transverse motion
  - To connect interior and exterior regions we invoke conservation of total energy
  - Since *d* is the only coordinate in the exterior, and since $E_{tot} - E_F$ is energy in the direction transverse to *d*, we cannot associate it with the kinetic energy, therefore we assign it to excitation energy of the FF

Work in progress by Bernard et al. is better approach, this is only a model to estimate the "dissipated" energy due to coupling between collective d.o.f.

Energy "dissipated" into excitation of fragments as a function of initial energy

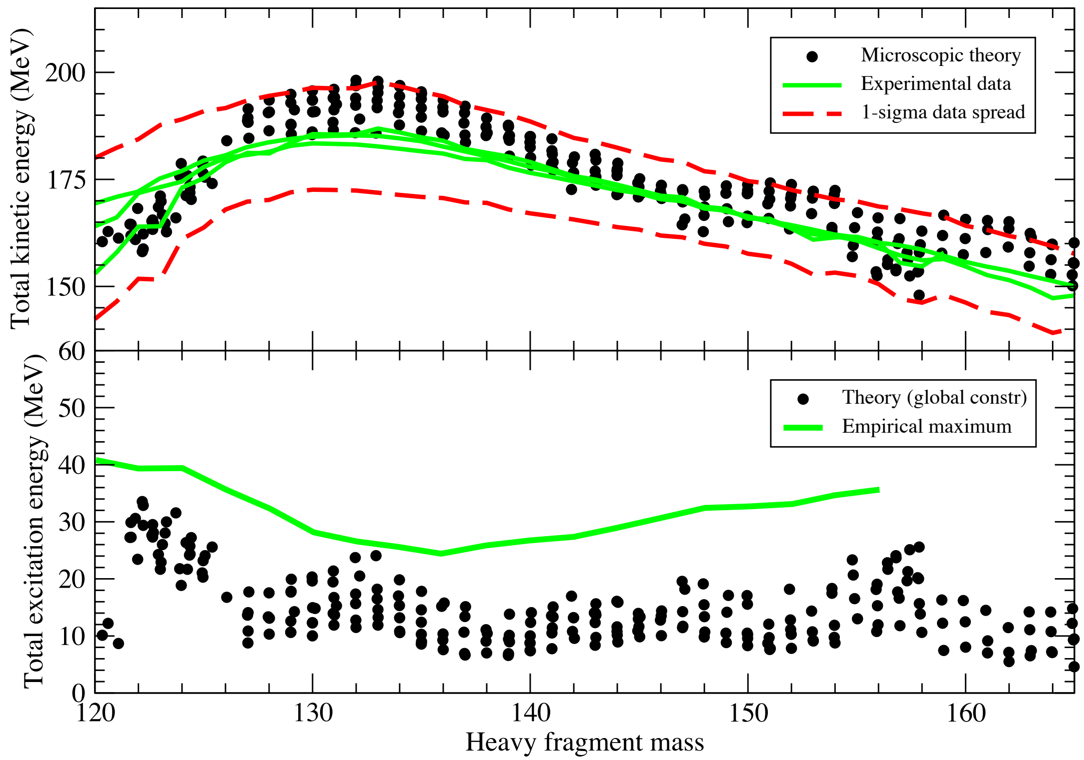


⇒ ~ 4 MeV dissipation, and that's just from Q_{20}-Q_{30} coupling: expect more energy dissipated via coupling between other (collective and intrinsic) d.o.f.!

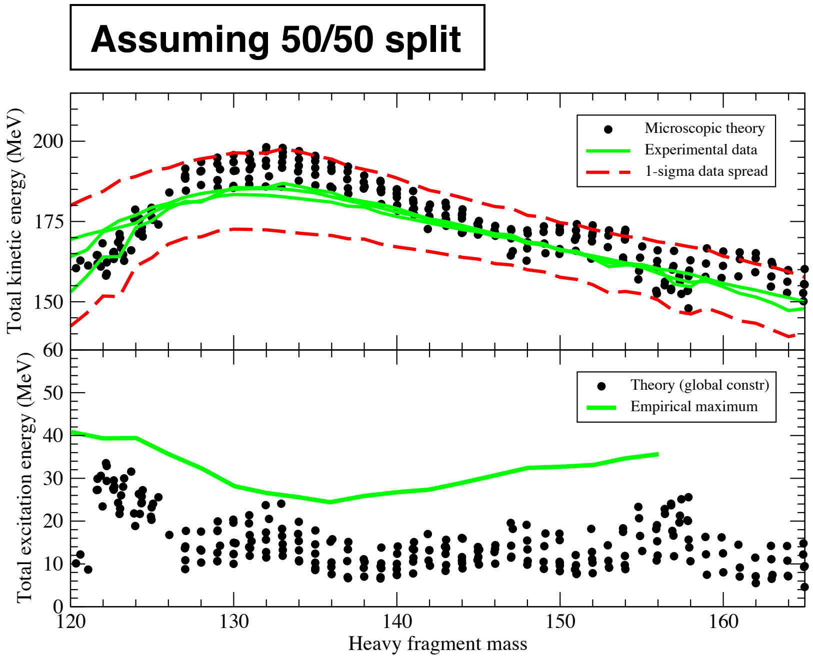
Calculated fragment kinetic and excitation energies for $^{239}Pu(n_{th},f)$

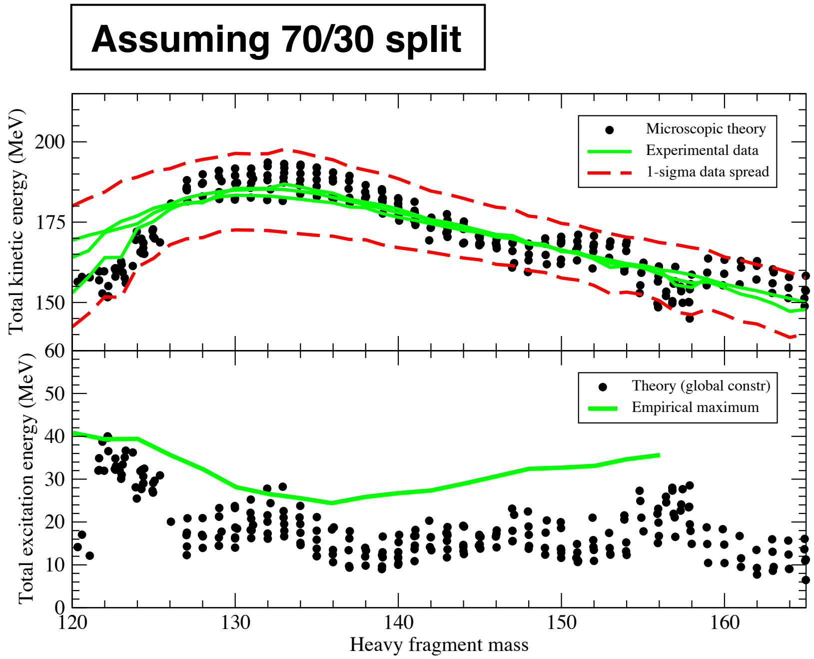
We have calculated ~ 8 MeV of pre-scission energy due to collective coupling, expect additional 2-3 MeV at least from collective-intrinsic (great unknown, see Bernard et al. PRC 84, 044308) ⇒ 50/50 split of saddle-to-scission energy between kinetic and excitation is not unreasonable (not too different from estimates by others, e.g. Gönnenwein):

Calculated TKE and TXE using our scission criterion & 50/50 split from dynamic contribution

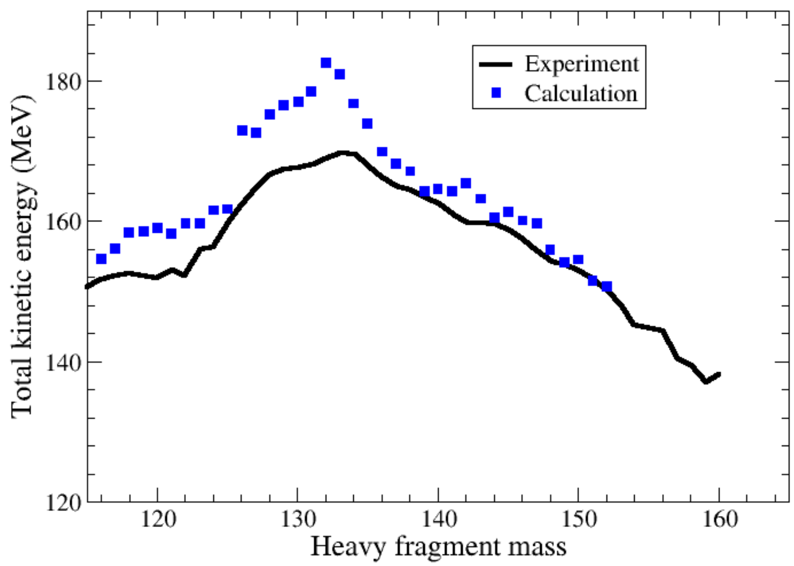


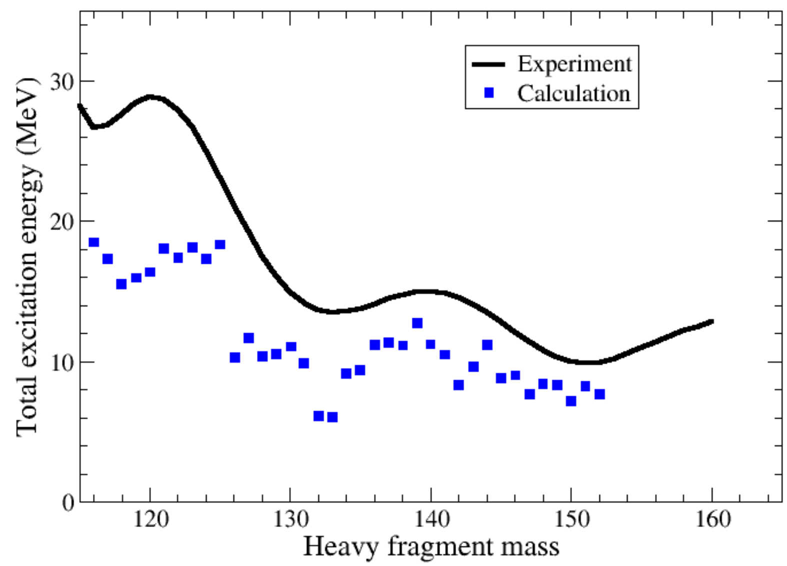
TKE and TXE assuming 70/30 split of excitation/kinetic





Results for ^{229}Th(n_{th},f): fragment kinetic and excitation energies





Starting from protons, neutrons, and effective interaction: Results consistent with experiment!

Conclusions: summary

- Ongoing program to develop a microscopic theory of fission, starting from protons, neutrons, and an effective interaction between them
- Starting point is mean-field approximation, followed by a hierarchical restoration of correlations beyond the mean field
- Progress in understanding scission within a quantum-mechanical framework
- Time-dependent formalism gives the dynamics of fission
- Today: calculation of multiple fission observables (fragment yields, fragment kinetic and excitation energies,…) within a single, self-consistent framework.
- Tomorrow: ?

Conclusions: future outlook

- There is active research in major aspects of the physics
  - Coupling between collective and intrinsic modes, and energy partition in fission
  - Fission at higher excitation energies
  - Number and nature of collective degrees of freedom near scission
  - Treatment of angular momentum in fission
  - Emission of scission neutrons
  - …

Additional work on microscopic theory of fission

- Scission configurations and their implication in fission-fragment angular momenta (L. Bonneau et al., Phys. Rev. C 75, 064313 (2007))
- Self-consistent calculations of fission barriers in the Fm region (M. Warda et al., Phys. Rev. C 66, 014310 (2002))
- Microscopic description of fission in uranium isotopes with the Gogny energy density functional (R. Rodríguez-Guzmán & L.M. Robledo, Phys. Rev. C 054310 (2014))
- Fission half-lives of superheavy nuclei in a microscopic approach (M. Warda & J. L. Egido, Phys. Rev. C 86, 014322 (2012))
- Microscopic calculation of ^{240}Pu scission with a finite-range effective force (W. Younes & D. Gogny, Phys. Rev. C 80, 054313 (2009))
- Fission barriers at high angular momentum and the ground-state rotational band of the nucleus 254No (J.L. Egido and L.M. Robledo, Phys. Rev. Lett. 85, 1198 (2000))

Additional work on microscopic theory of fission (cont)

- Microscopic study of 240Pu: Mean field and beyond (M. Bender et al., Phys. Rev. C 70, 054304 (2004))
- Microscopic transport theory of nuclear processes (K. Dietrich et al., Nucl. Phys. A832, 249 (2010))

Useful reviews

- J.F. Berger, “La Fission: de la phénoménologie à la théorie”, Ecole Joliot-Curie (2006) (in French)
- H.J. Krappe and K. Pomorski, “Theory of Nuclear Fission”, Lecture Notes in Physics 838 (2012)
- J.F. Berger “Approches de champ moyen et au dela”, Ecole Joliot-Curie (1991) (in French)
- M. Bender et al., “Self-consistent mean-field models for nuclear structure”, Rev. Mod. Phys. 75, 121 (2003)