Theories of Fission Product Yields

FIESTA Summer School

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Introduction

- Historical Remarks
- Some Definitions
- The Big Picture

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Experimental Discovery of Nuclear Fission

Hahn Strassman Meitner

Hahn's Worktable

- 1939: experimental discovery of neutron-induced fission

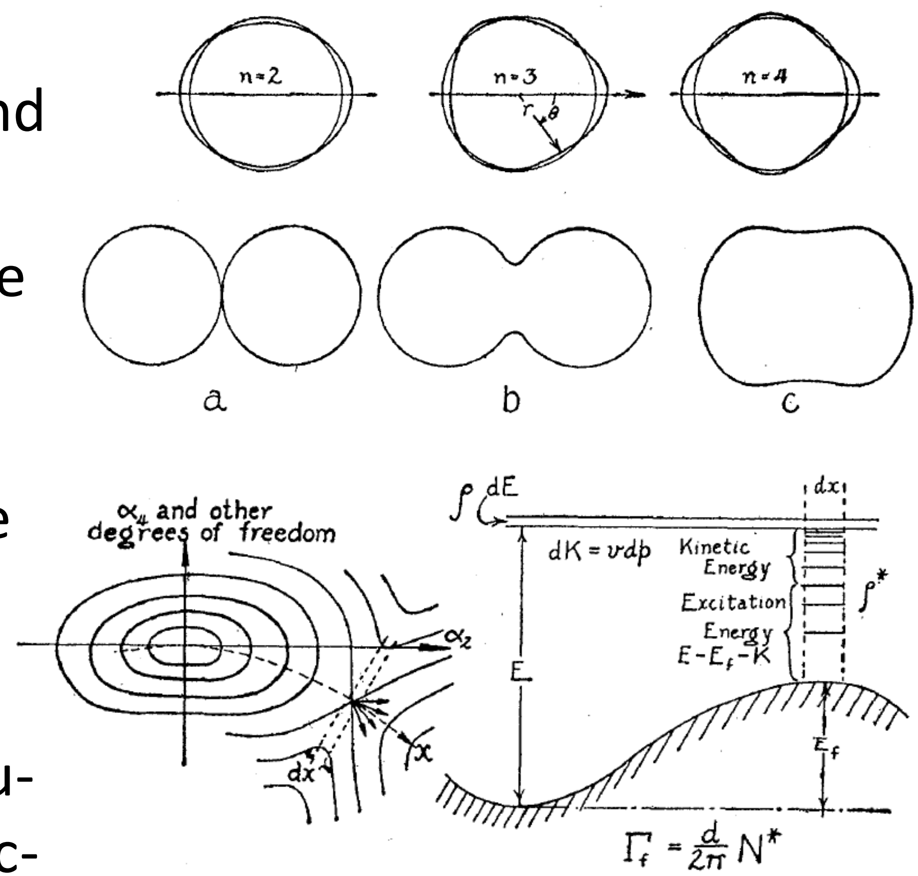
that Hahn and Strassmann were forced to conclude that *isotopes of barium* ($Z = 56$) *are formed as a consequence of the bombardment of uranium* ($Z = 92$) *with neutrons.* L. Meitner, Nature **3615**, 239 (1939).

On the basis, however, of present ideas about the behaviour of heavy nuclei[6], an entirely different and essentially classical picture of these new disintegration processes suggests itself. On account of their close packing and strong energy exchange, the particles in a heavy nucleus would be expected to move in a collective way which has some resemblance to the movement of a liquid drop. If the movement is made sufficiently violent by adding energy, such a drop may divide itself into two smaller drops.

- 1940: experimental discovery of spontaneous fission by K.A. Petrzhak and G.N. Flerov

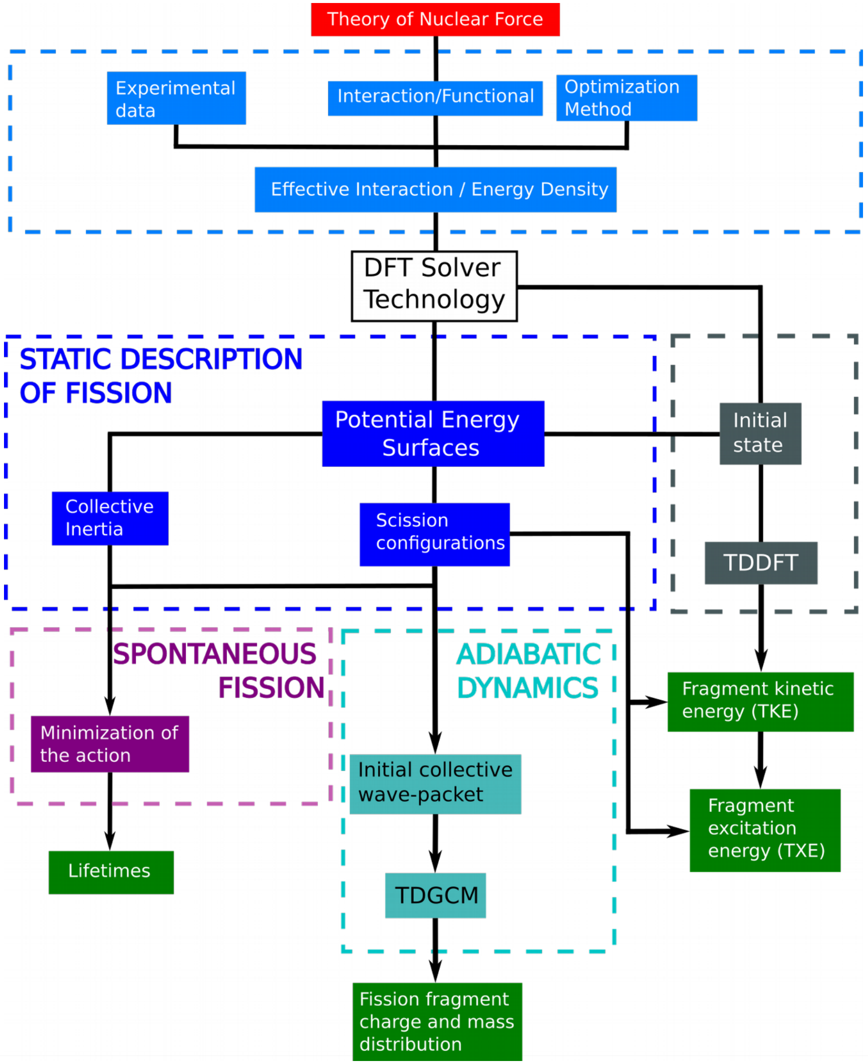
Fission: A Large Amplitude Collective Motion

- Induced fission as a two-step process: formation of a compound nucleus followed by its decay
- Semi-classical process that can be described by a set of collective variables (=deformations)
- Separate collective motion of the nucleus as a whole and intrinsic excitations of its constituents
- Adiabatic approximation: the coupling between intrinsic and collective can be neglected



Theorist's TODO List

- Choose collective variables
- Compute energy as a function of collective variables
- Compute dynamical evolution through that space
  - Quantum tunneling for spontaneous fission
  - Quantum collective flow for fission fragment distributions
- Alternatives
  - Statistical model
  - Real-time dynamics for single fission events



Nuclear static properties in the collective space

- Macroscopic-Microscopic Models (4)
- Nuclear Density Functional Theory (4)
- The Concept of Scission (3)

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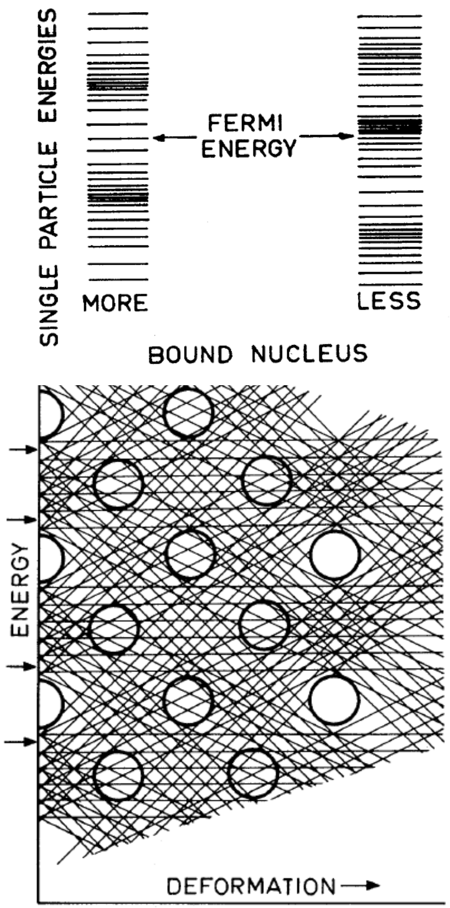
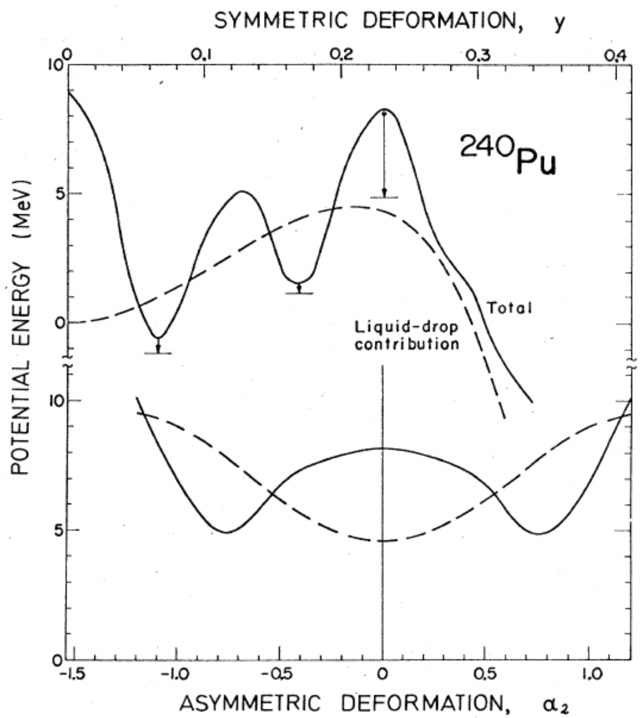
Macroscopic-microscopic Models (1/4)

Introduction





- Take into account nucleon degrees of freedom
  - Shell correction coming from the distribution of single-particle levels
  - Pairing correction to mock up the effect of residual interactions
- Extensions to finite angular momentum or temperature are also available

In the macroscopic-microscopic approach, the basic degrees of freedom are the single-particle states and the nuclear deformations, and the equation of motion is the Schrödinger equation

Macroscopic-microscopic Models (2/4)

Components of the Total Energy

- Total energy is written

$$E(\boldsymbol{q}) = E_{\mathrm{mac}}(\boldsymbol{q}) + \delta R_{\mathrm{shell}}(\boldsymbol{q}) + \delta R_{\mathrm{pair}}(\boldsymbol{q})$$

- Macroscopic liquid drop energy

$$E_{\mathrm{mac}}(\boldsymbol{q}) = E_{\mathrm{vol}} + E_{\mathrm{surf}}(\boldsymbol{q}) + E_{\mathrm{asym}}(\boldsymbol{q}) + E_{\mathrm{Coul.}}(\boldsymbol{q})$$

- Shell correction

$$\delta R_{\mathrm{shell}}(\boldsymbol{q}) = \sum_n e_n - \left\langle \sum_n e_n \right\rangle$$

- Pairing correction

$$\delta R_{\mathrm{pair}}(\boldsymbol{q}) = E_{\mathrm{pair}} - \tilde{E}_{\mathrm{pair}}$$

- Shell and pairing corrections require a set of single-particle energies e_n: need to solve the Schrödinger equation

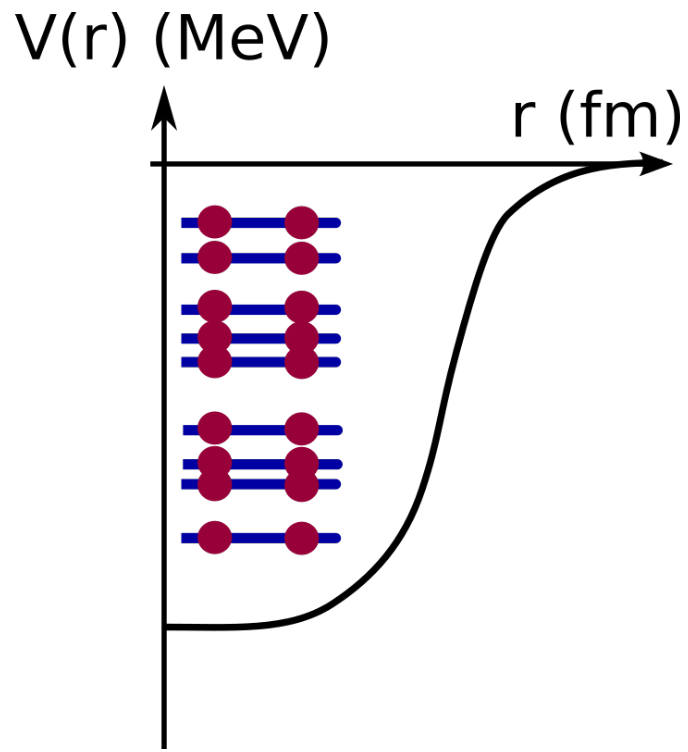
Macroscopic-microscopic Models (3/4)

Single-Particle Degrees of Freedom

- (One-body) Schrödinger equation

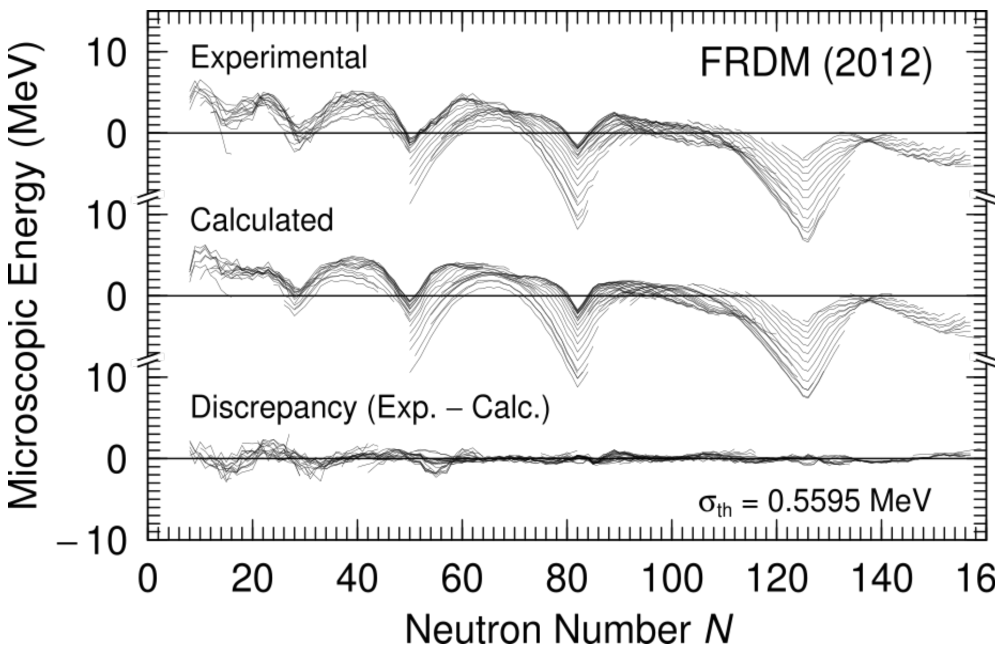
$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2 + V_{\boldsymbol{q}}(\boldsymbol{r})\right]\varphi_n(\boldsymbol{r}) = e_n\varphi_n(\boldsymbol{r})$$

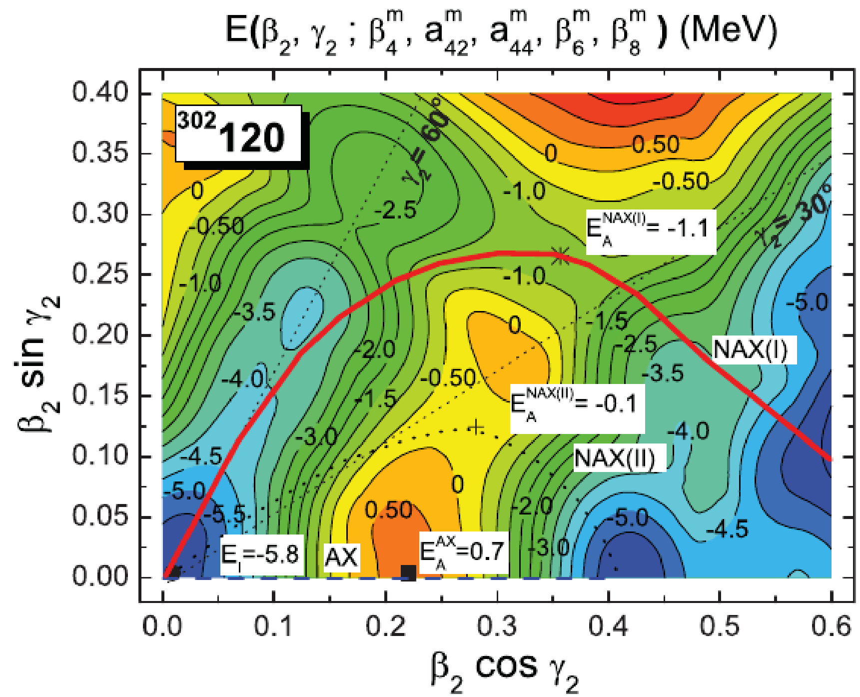
- Mean-field potential can be Nilsson, Woods-Saxon, Folded-Yukawa, etc.
- Solve BCS equation (for example) to compute occupation of s.p. states and extract pairing energy
- Collective variables are deformations that define the shape of the potential



Macroscopic-microscopic Models (4/4)

Examples





- The macroscopic-microscopic model can be applied to ground-state properties, e.g., masses
- Given a set of collective variables, we can calculate the potential energy surface, that is, the function *E(**q**)*

Nuclear Density Functional Theory (1/4)

Introduction

- Describe fission as emerging from nuclear forces and quantum many-body effects
- (Many-body) Schrödinger equation for the nucleus

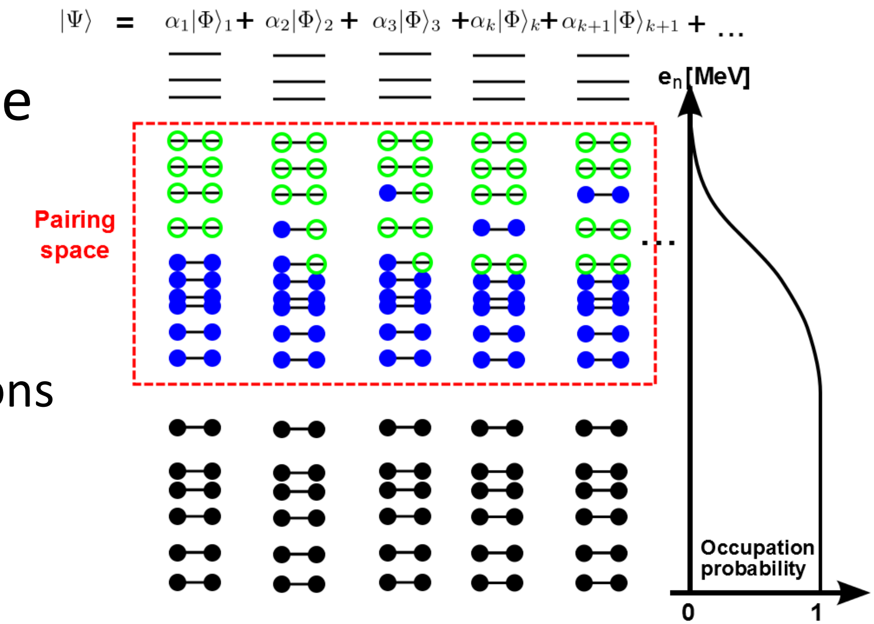
Exact many-body Hamiltonian, e.g., chiral effective field theory → $$\hat{H}|\Psi_n\rangle = E_n|\Psi_n\rangle$$ ← *Exact many-body wavefunctions with all correlations built-in*

- Why is it impossible for heavy nuclei (at least in this century)?
  - We do not know the exact nuclear Hamiltonian, only have (good) approximations of it that involve 2-, 3- and now 4-body forces
  - The exact wavefunction depends on 3A coordinates, 3A momenta, and A spins: computational requirements for heavy nuclei are out of this world (current limit: A ≤ 16 and heavier closed-shells nuclei)
- How to simplify the problem while keeping as much quantum mechanics and information about nuclear forces?

Nuclear Density Functional Theory (2/4)

From reference states to densities

- Replace the (unobtainable) exact wave function by a simpler form, the reference state
  - Independent particle model: Slater determinant, an (antisymmetrized) product of single-particle wave functions
  - DFT: HFB vacuum, a very particular superposition of Slater determinants
- Replace exact Hamiltonian with effective one such that energy computed with reference state is OK
- Energy becomes a functional of density of particles and pairing tensor



$$\langle\Phi|\hat{H}_{\text{eff.}}|\Phi\rangle \rightarrow E[\rho,\kappa]$$

Nuclear Density Functional Theory (3/4)

Static nuclear properties with reference states

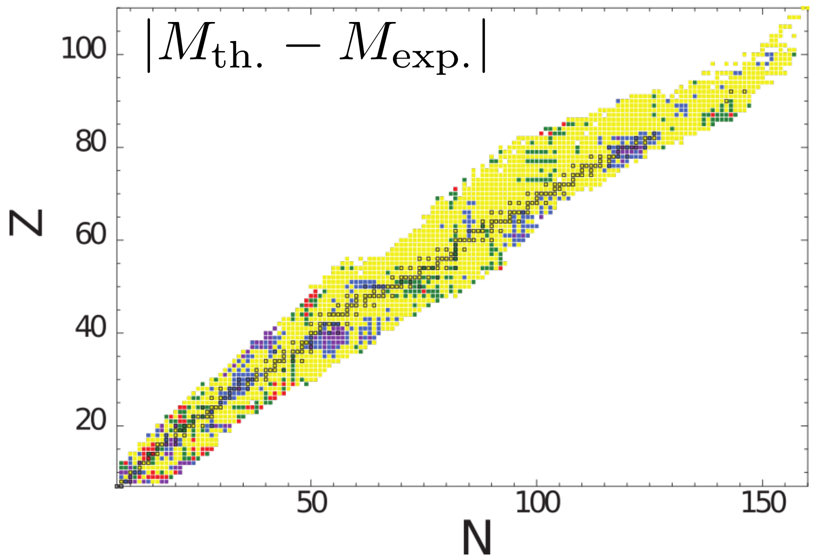
- Form of the energy functional chosen by physicists, often guided by characteristics of nuclear forces (central force, spin-orbit, tensor, etc.): Skyrme, Gogny, etc.
- Variational principle: determine the actual densities of the nucleus by requiring the energy is minimal with respect to their variations
  - Resulting equation is called HFB equation (Hartree-Fock-Bogoliubov)
  - Solving the equation gives densities and characteristics of the reference state
- Any observable can be computed knowing the density

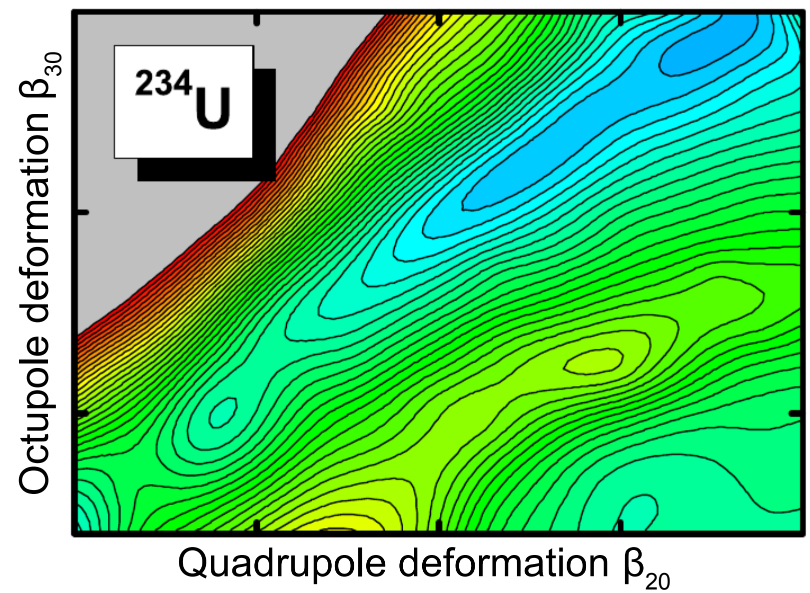
$$\langle r^2 \rangle = \int d^3\boldsymbol{r}\ \rho(\boldsymbol{r})\boldsymbol{r}^2$$

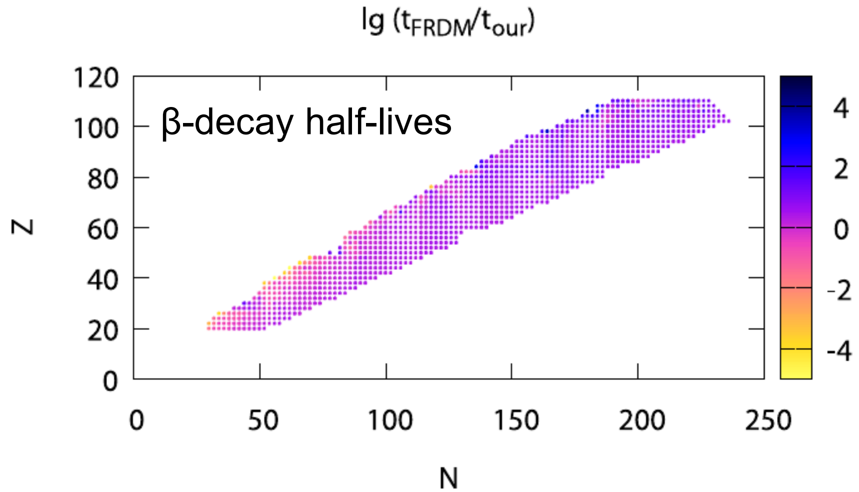
- One can compute potential energy surfaces by solving the HFB equation with constraints on the value of the collective variables

Nuclear Density Functional Theory (4/4)

Examples



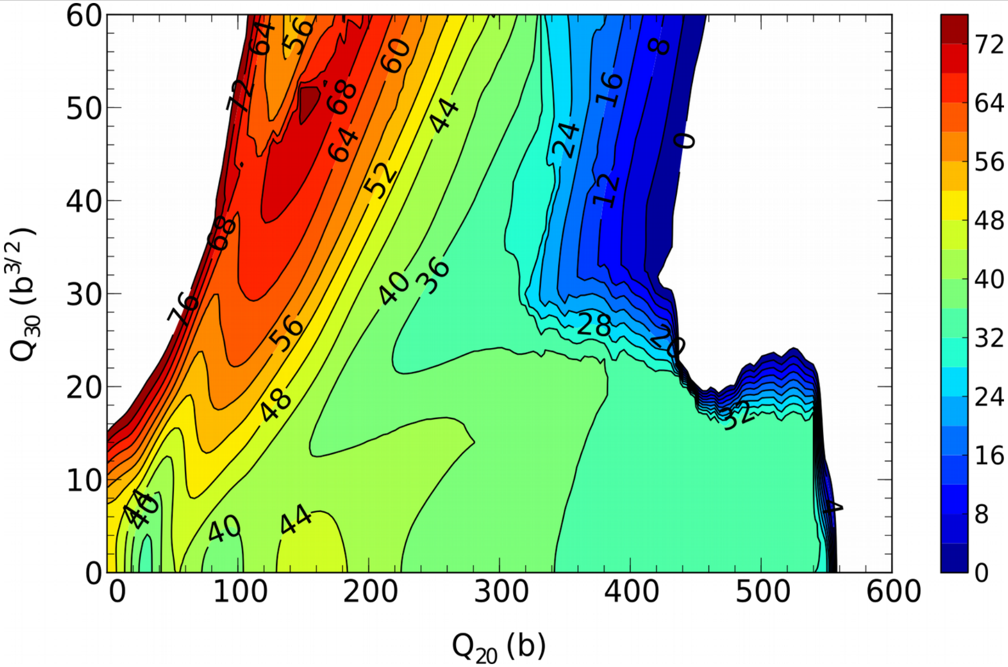


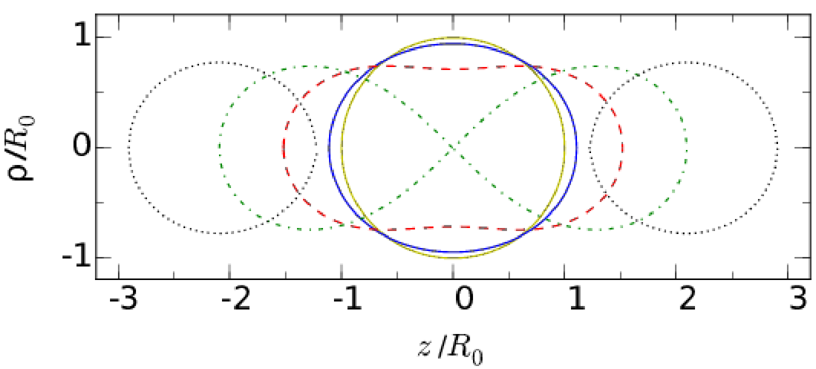


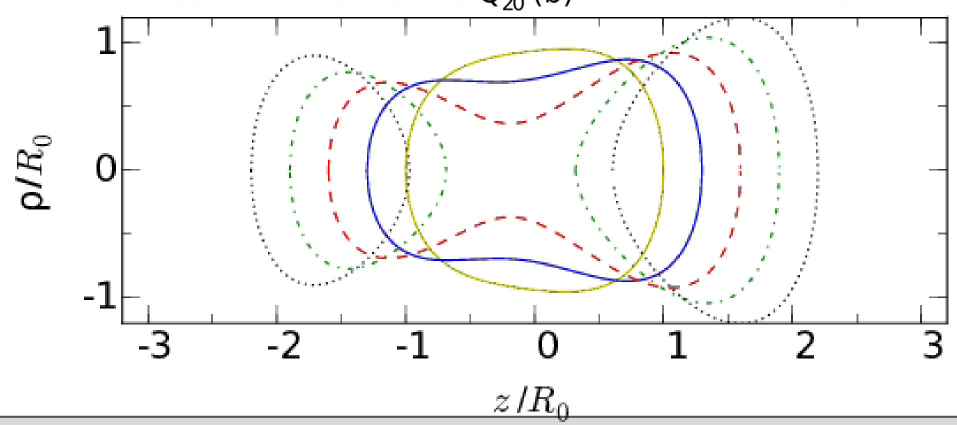
- DFT can now be applied to g.s. properties (masses), decays (beta-decay)
- Potential energy surfaces can be computed easily

Concept of Scission (1/3)
Introduction

- The scission line distinguishes regions of the PES where the nucleus is whole and where it has split in two fragments
  - Macro-micro: can be built-in the shape parametrization
  - DFT: often identified as a discontinuity



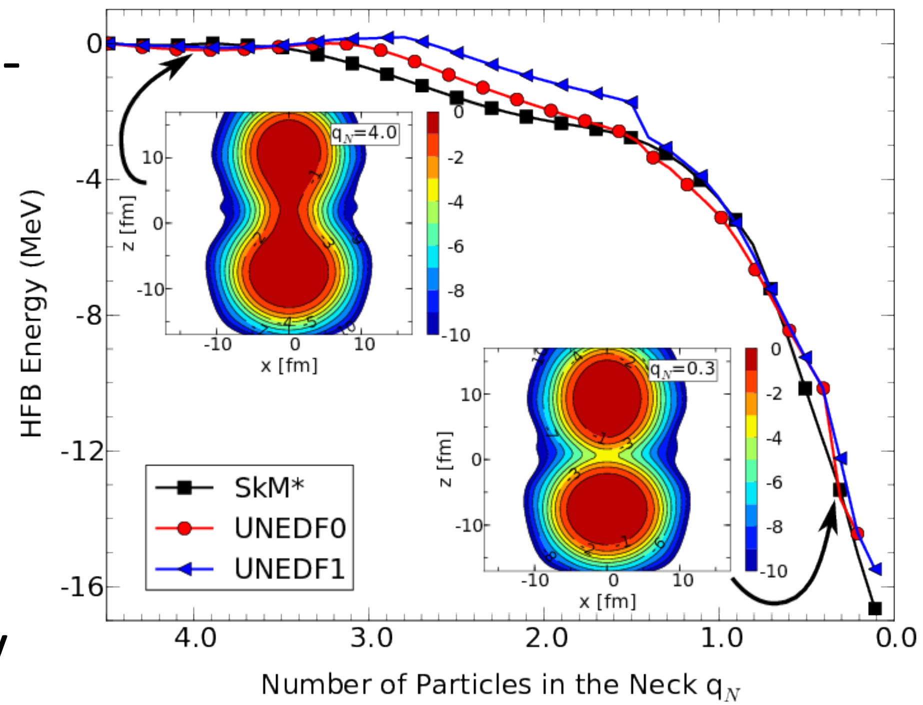




Concept of Scission (2/3)

Continuous scission

- Sharp, geometric scission unrealistic
  - Coulomb forces take over nuclear forces before neck vanish
  - DFT: scission often viewed as discontinuity but only because finite number of collective variables
- More realistic descriptions imply scission (radius, density, etc.) becomes a parameter of the calculation

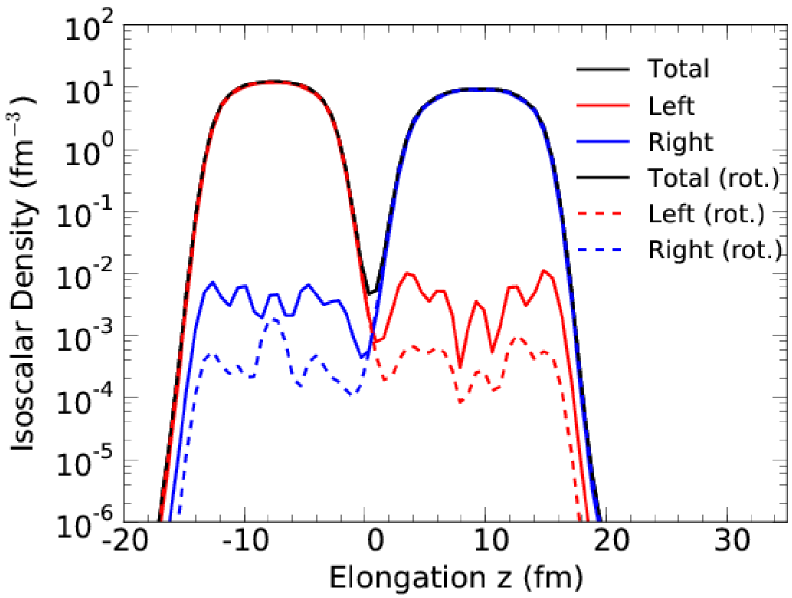


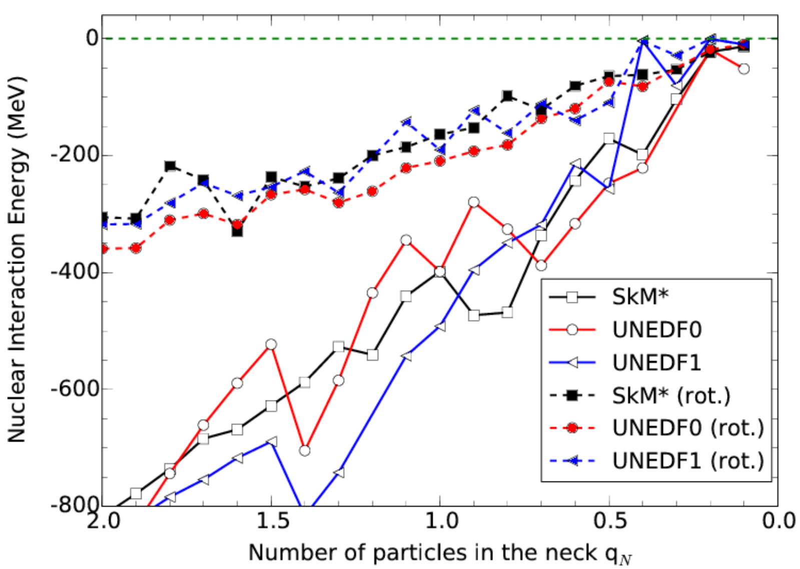
$$\langle \hat{Q}_N \rangle = \int d^3\mathbf{r}\ \rho(\mathbf{r}) e^{-\left(\frac{z - z_N}{a}\right)^2}$$

Concept of Scission (3/3)

Scission and quantum entanglement

- Simple, user-defined criteria for scission often ignore
  - Quantum nature of fission fragments and neck region: antisymmetry
  - Finite-range of nuclear and Coulomb forces
- Adiabatic theory not adapted to describe dynamical, non-equilib-rium process such as scission





Fission Dynamics

- Scission Point Model (1)
- Classical Dynamics (2)
- Quantum Dynamics – TDGCM (3)
- Quantum Dynamics – TDDFT (3)

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The Scission Point Model

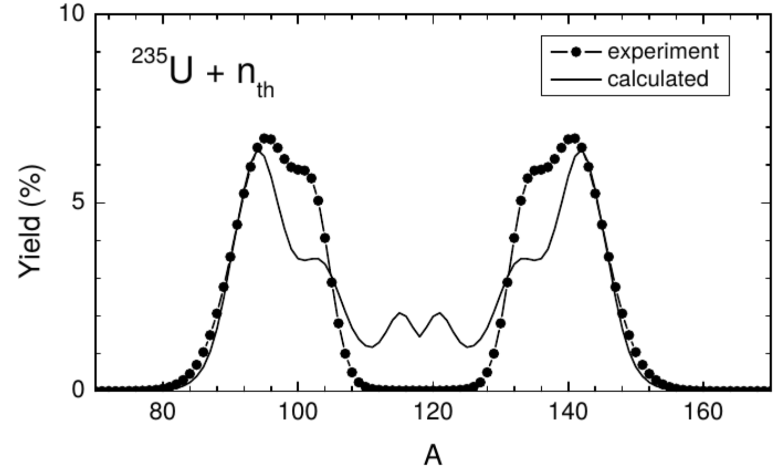
Statistical Approximation to Fission Dynamic

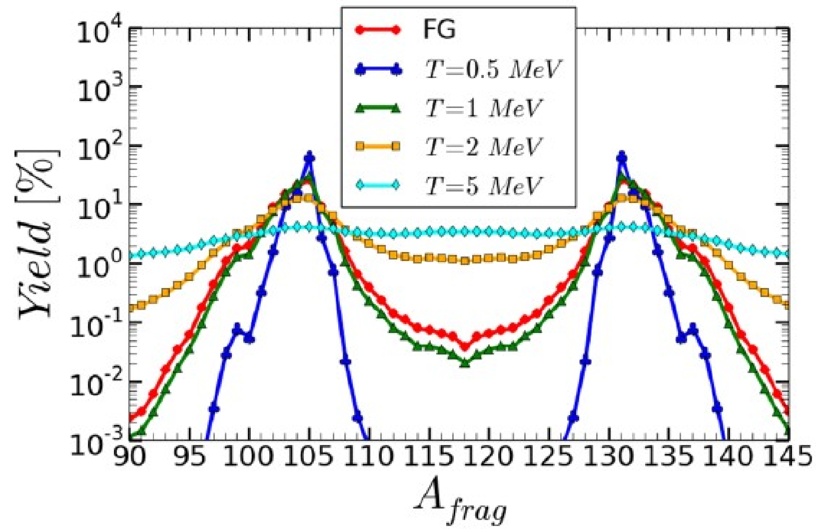
- Static picture exclusively based on the structure of the potential energy surface at scission (including the fragment characteristics)
- Probability of fission is simply related to (Wilkins)

$$\propto \int d\boldsymbol{q}_1 \int d\boldsymbol{q}_2 e^{-V(\boldsymbol{q}_1,\boldsymbol{q}_2;\alpha)/T}$$

or the level densities of the two fragments (SPY)

$$\propto \int d\boldsymbol{q}_1 \int d\boldsymbol{q}_2 \rho_1(\boldsymbol{q}_1;\alpha)\rho_2(\boldsymbol{q}_2;\alpha)$$





Classical Dynamics (1/2)

Langevin equations

- How to extract fission product yields from the knowledge of the potential energy surface?
  - Analogy with classical theory of diffusion
  - Collective variable = generalized coordinate
  - Define related momentum
- Langevin equations

$$\dot{q}_\alpha = \sum_\beta B_{\alpha\beta} p_\beta ,$$

Friction tensor

Random force

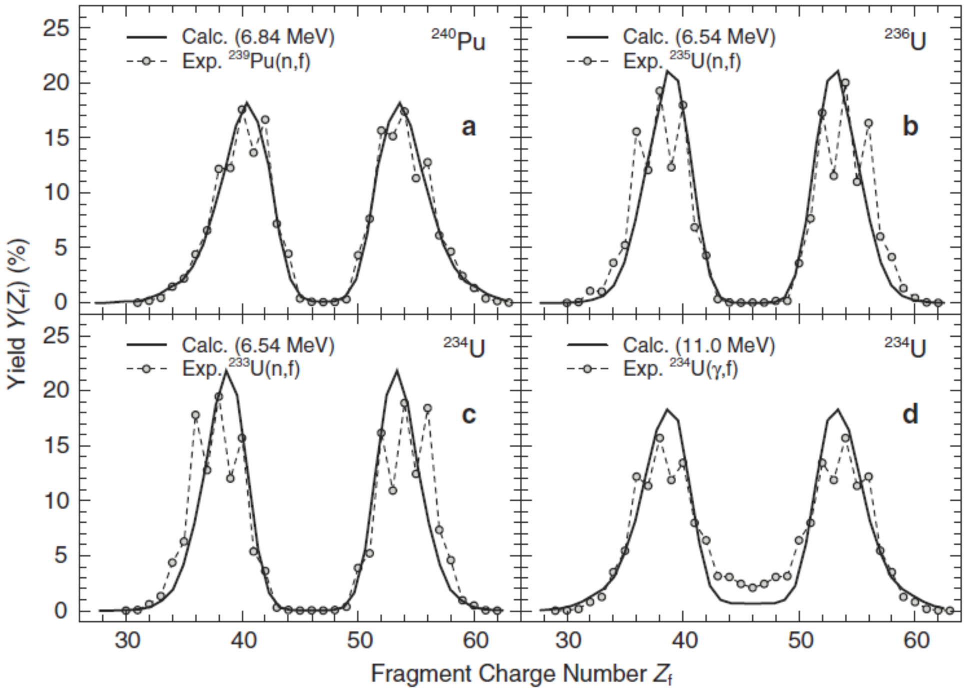
$$\dot{p}_\alpha = -\sum_{\beta\gamma} \Gamma_{\alpha\beta} B_{\beta\gamma} p_\gamma + \sum_\beta \Theta_{\alpha\beta} \xi_\beta(t) - \frac{1}{2} \sum_{\beta\gamma} \frac{\partial B_{\beta\gamma}}{\partial q_\alpha} p_\beta p_\gamma - \frac{\partial V}{\partial q_\alpha}$$

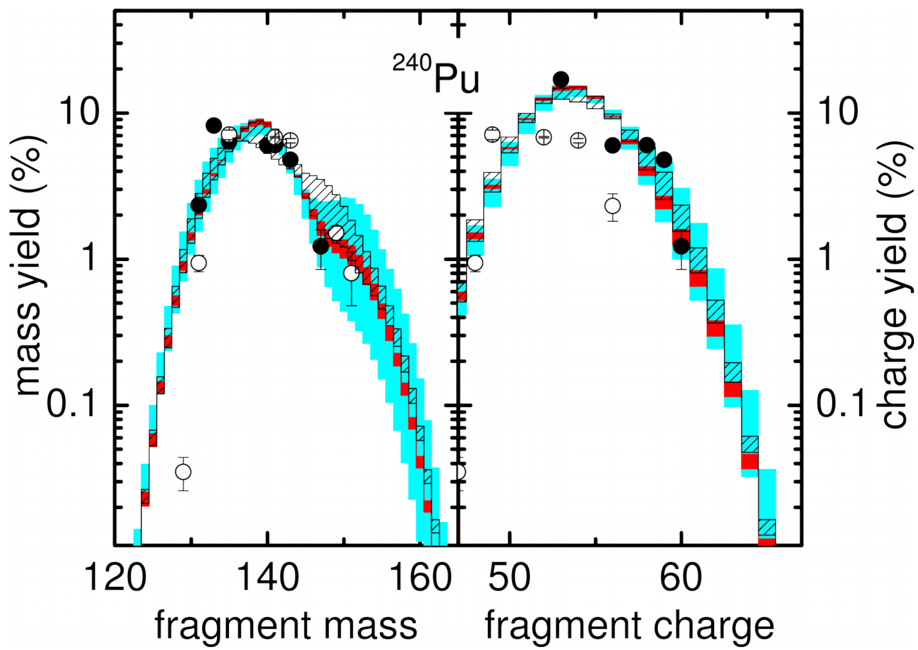
Fluctuation-dissipation theorem

$$\sum_k \Theta_{ik} \Theta_{kj} = \Gamma_{ij} T$$

Classical Dynamics (2/2)

Practical examples





- Start beyond the saddle point (or close enough)
- Build trajectories through the collective space by generating at each step the needed random variable
- Enough trajectories (in the thousands) allow reconstructing FPY

Quantum Dynamics - TDGCM (1/3)

Computing the flow of probability in the collective space

- Ansatz for the time-dependent many-body wave function

$$|\Psi(t)\rangle = \int d\mathbf{q}\, f(\mathbf{q},t)|\Phi(\mathbf{q})\rangle$$

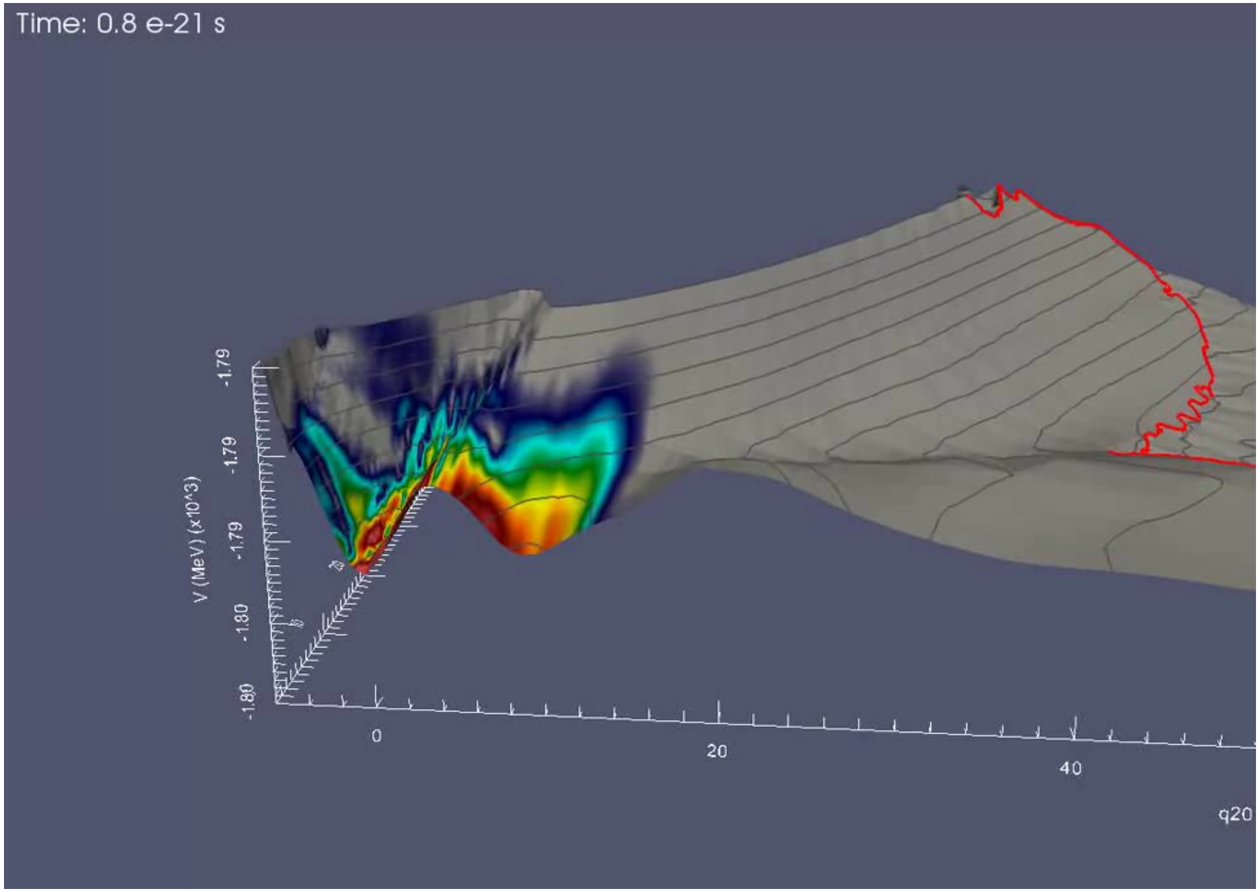
- Minimization of the time-dependent quantum mechanical action + ansatz + Gaussian overlap approximation + some patience

$$i\hbar\frac{\partial}{\partial t}g(\mathbf{q},t) = \left[-\frac{\hbar^2}{2}\sum_{kl}\frac{\partial}{\partial q_k}B_{kl}\frac{\partial}{\partial q_l} + V(\mathbf{q})\right]g(\mathbf{q},t)$$

- Interpretation
  - $g(\mathbf{q},t)$ is probability amplitude to be at point **q** at time t
  - Related probability current
  - Flux of probability current through scission line gives yields

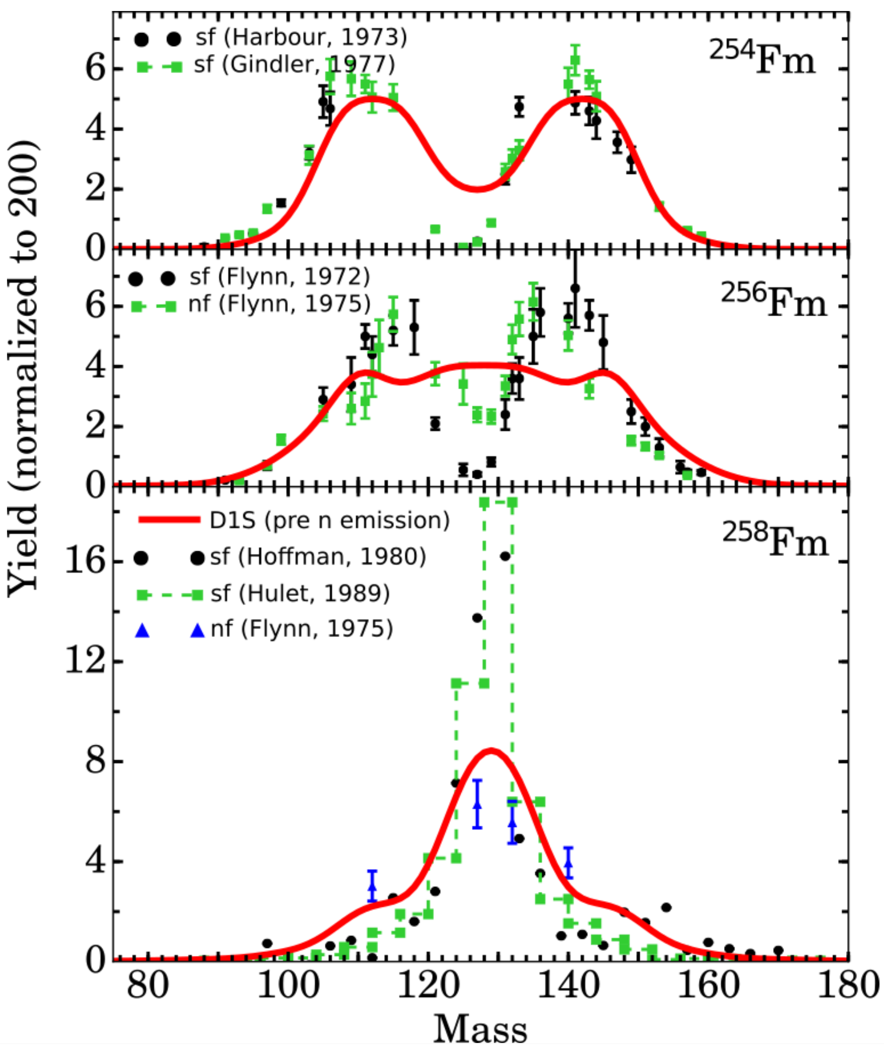
Quantum Dynamics - TDGCM (2/3)

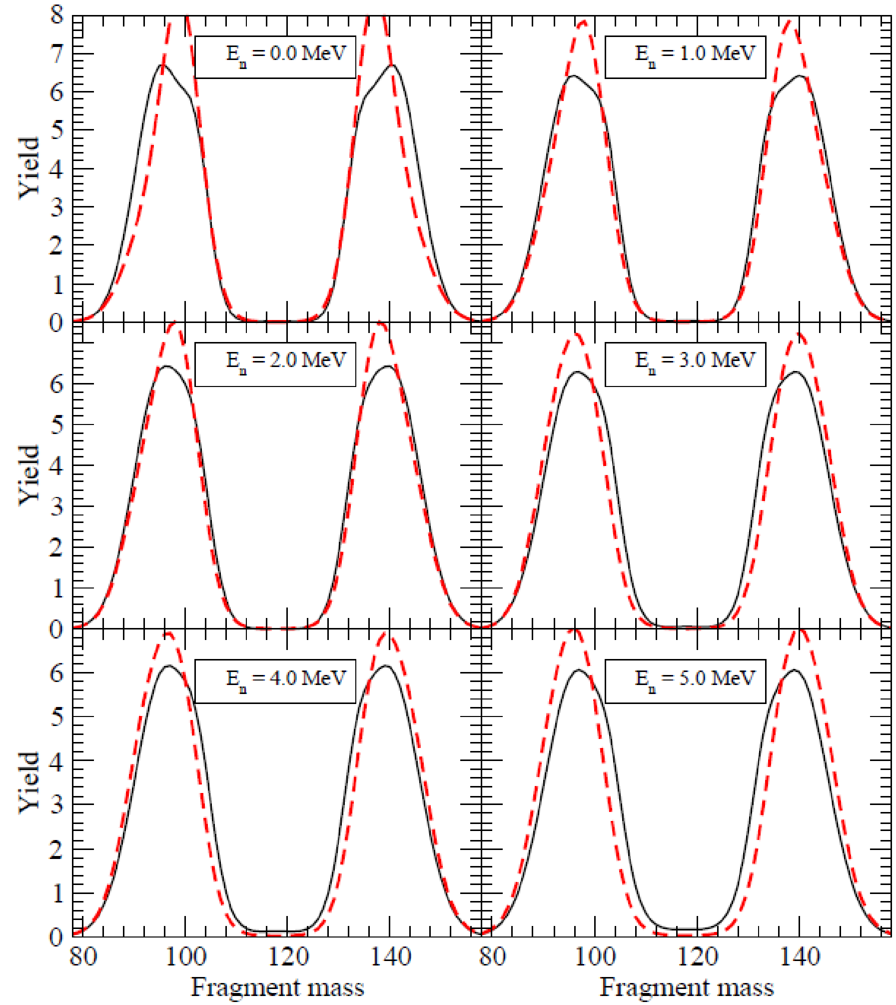
Example: TDGCM Evolution



Quantum Dynamics – TDGCM (3/3)

Examples: Fission Product Yield Calculations





Quantum Dynamics – TDDFT (1/3)

Brief Introduction

- Main limitation of Langevin and TDGCM: adiabaticity is built-in
  - Need to precompute potential energy surfaces (costly)
  - Invoke arbitrary criteria for scission
  - Does not (easily) include dissipation = exchange between intrinsic (=single-particle) and collective degrees of freedom
- Solution: Generalize DFT to time-dependent processes
- Start from time-dependent many-body Schrödinger equation

$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}|\Psi(t)\rangle$$

- Insert approximation that many-body state is q.p. vacuum at all time

$$i\hbar\frac{\partial\mathcal{R}}{\partial t} = \left[\mathcal{H}, \mathcal{R}\right]$$

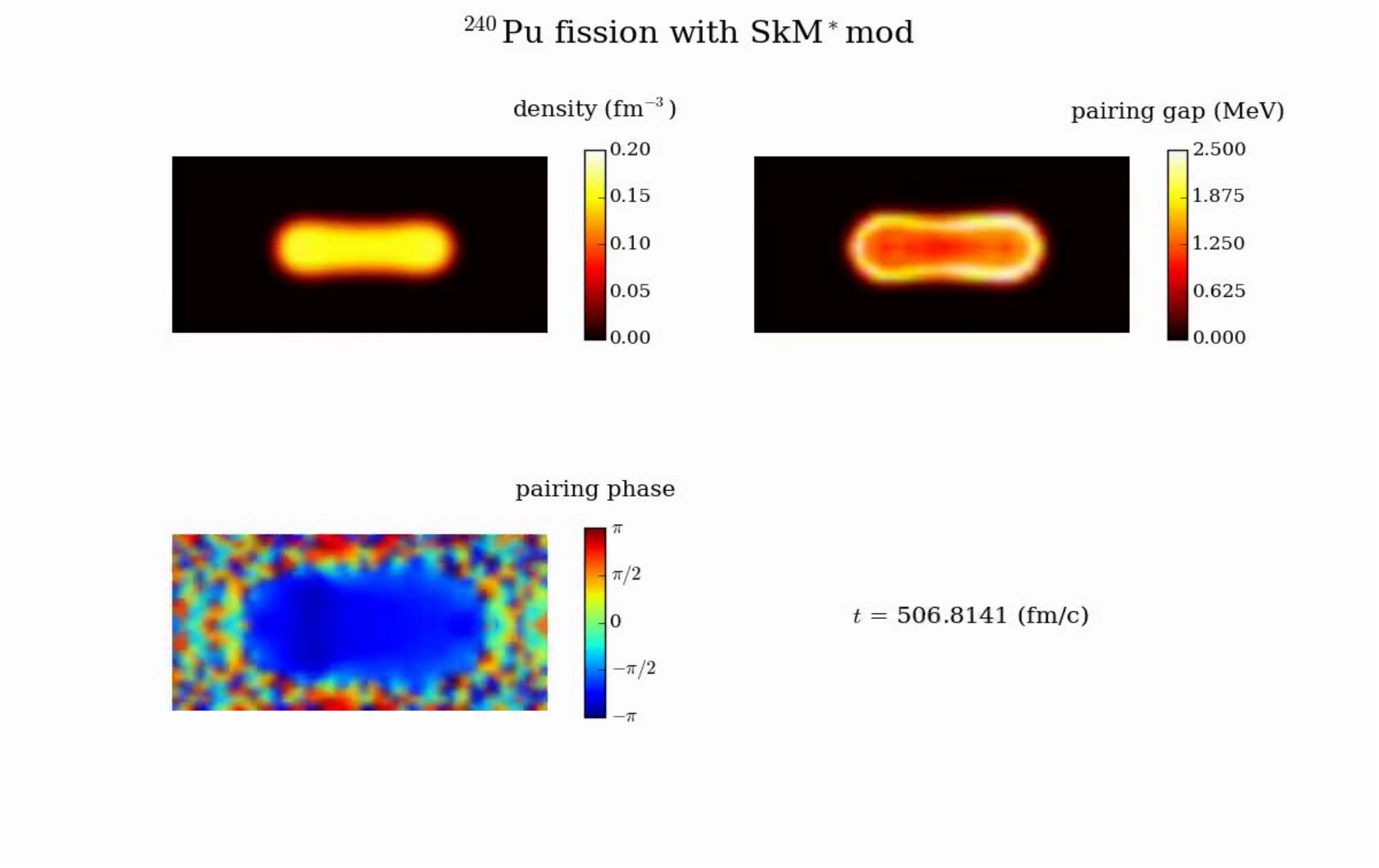
Quantum Dynamics – TDDFT (2/3)

Advantages and Limitations

- Advantages
  - TDDFT does not require adiabaticity, total energy is conserved: diabatic excitation of s.p./q.p. states
  - Dynamic shape evolution: normal and pairing vibrations, giant resonances
  - Produces ‘naturally’ excited fission fragments
- Limitations
  - Computational cost is enormous (especially for TDHFB)
  - Nucleus cannot tunnel through (semi-classical): not adapted to SF
  - Need HFB solver in coordinate space
- Computing FPY from TDDFT by sampling trajectories is in principle possible but would require computational resources at or beyond exascale (100x what we have now)

Quantum Dynamics – TDDFT (3/3)

Examples



Conclusions

- Navigating the zoo of methods
- Perspectives

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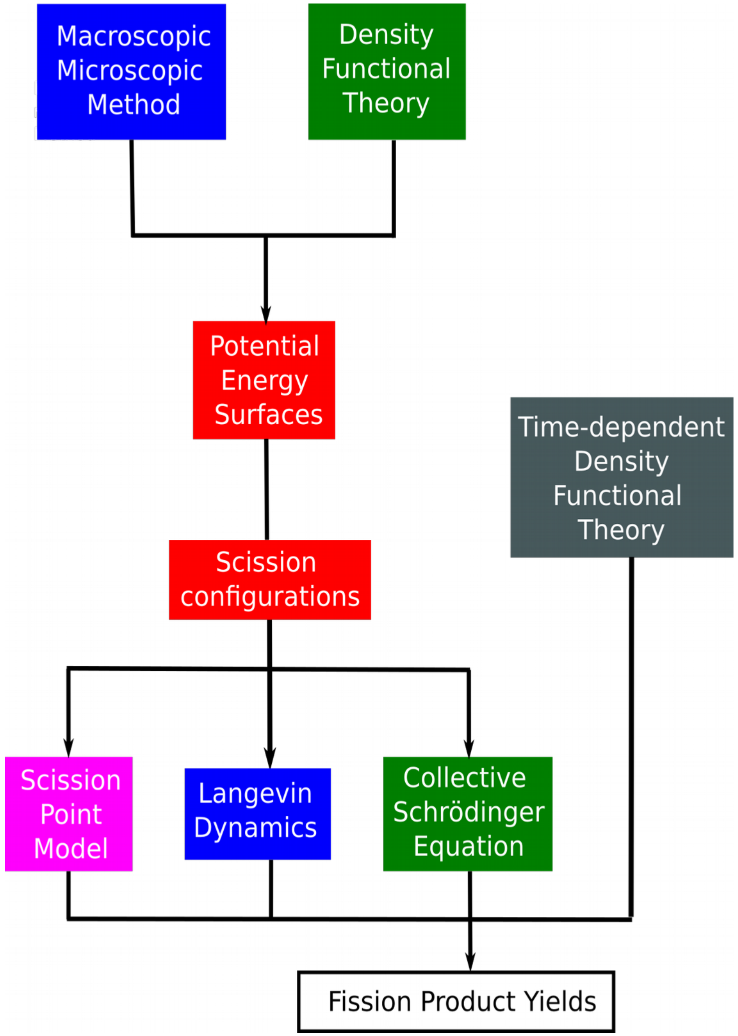
A Bird's View

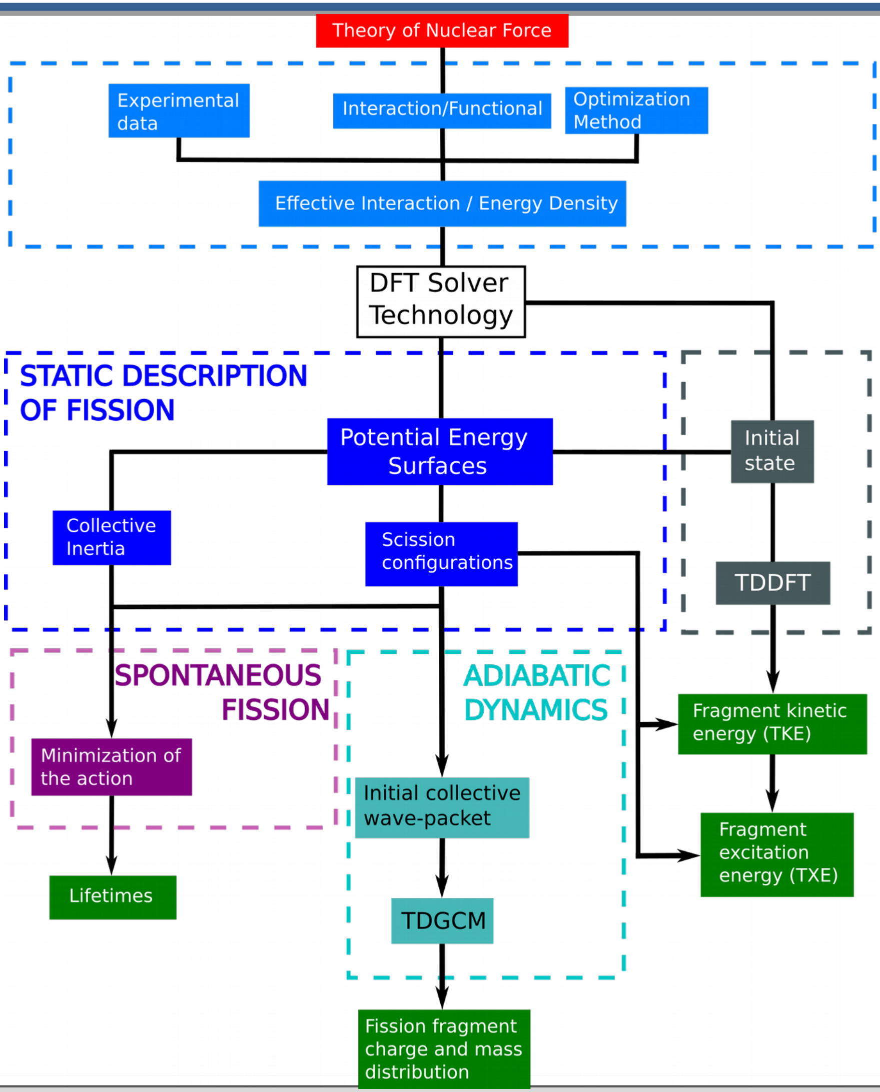
Elements of comparisons of different approaches

	Quantum	Description	Adiabaticity	Observable	Computational cost
Scission point model	Half	Static	Yes	Fission yields	Low
Macro-micro + Langevin	Half	Static + dynamic	Yes	Fission events	Low
DFT + TDGCM	Full	Static + dynamic	Yes	Fission yields	Moderate-high
TDDFT	Full	Dynamic	No	Fission events	Very high

A Bird's View

Elements of comparisons of different approaches





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