A Microscopic Theory of Fission (part I)

FIESTA 2014 Summer School

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Physical and Life Sciences

Lawrence Livermore National Laboratory

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"*it is conceivable that the nucleus breaks up into several large fragments, which would of course be isotopes of known elements but would not be neighbors of the irradiated element.*" – Ida Noddak (1934)

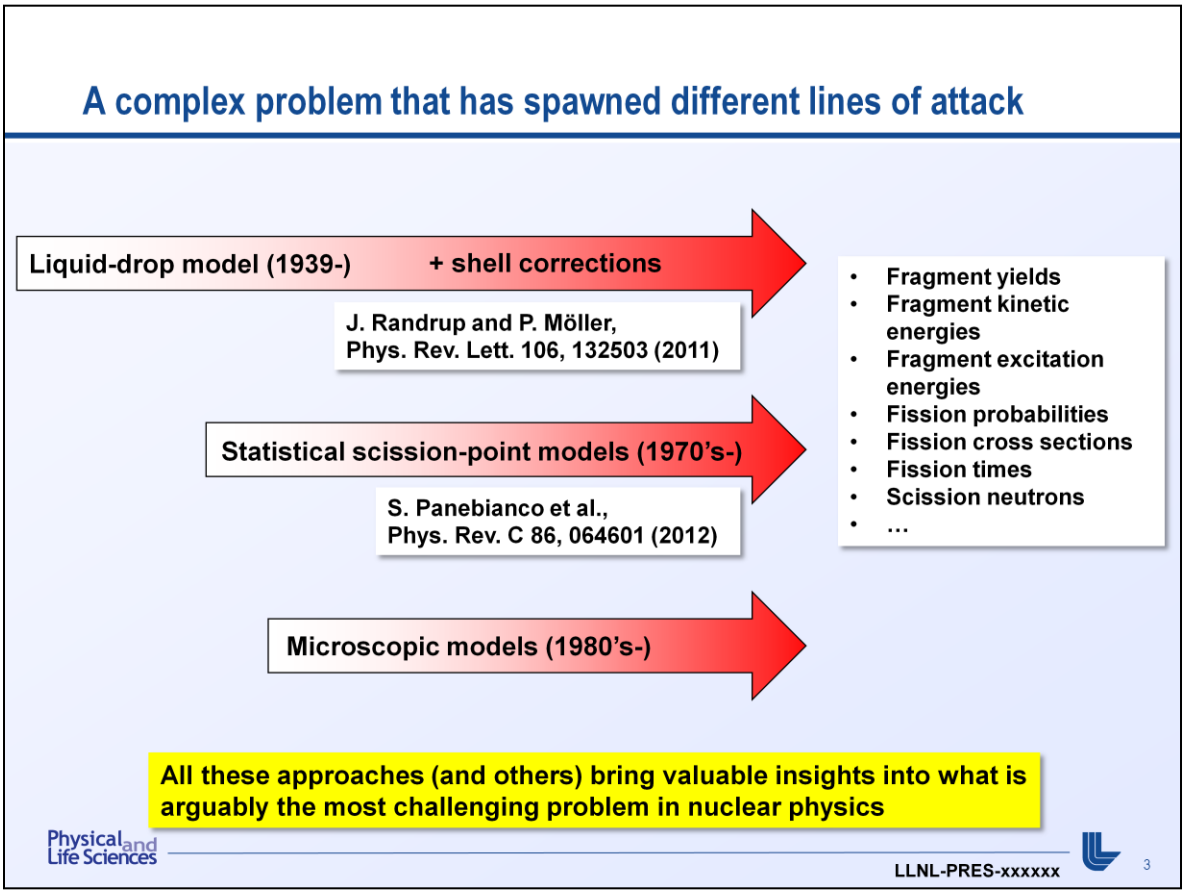
80 years later, there is still a lot we don't understand about fission!

"Problems worthy of attack prove their worth by hitting back" – Piet Hein

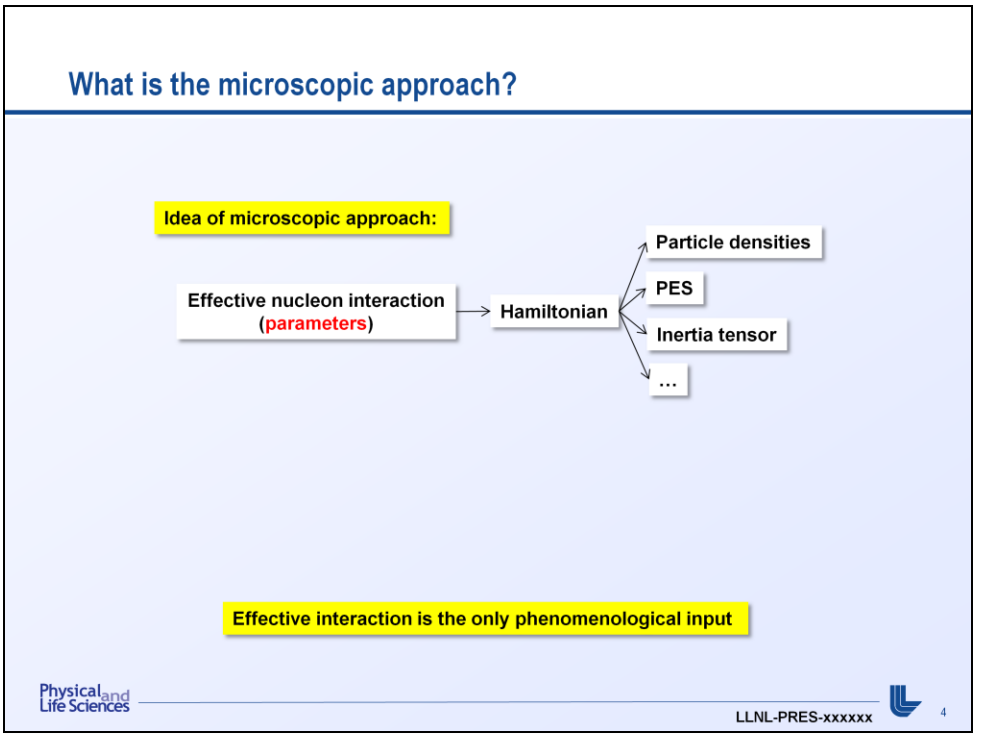
The story of fission begins in 1934 with these words from Ida Noddack, a German chemist and physicist. She was criticizing Fermi's assertion that he had created transuranic elements by neutron bombardment of uranium.

Unfortunately her remarks were largely ignored, and it wasn't until 1938 that she would be proven right by Otto Hahn and Fritz Strassmann who showed by chemical analysis that the presumed transuranic elements were in fact isotopes of barium.

That was 80 years ago, and there is still a lot we don't yet understand about fission!



- Many approaches have been developed to calculate fission observables of interest
- Each of these approaches has a well-established history of successes through the years
- These different approaches are not mutually exclusive. For example scission-point models, which were developed specifically to calculate fission-fragment properties, have used ingredients from both Liquid-drop + shell correction and microscopic approaches
- For an overview and comparison of different approaches to fission, see the slide "Useful reviews" at the end of this talk



- At the heart of the microscopic approach to fission is the self-consistent construction of the nuclear Hamiltonian from effective (i.e., in-medium) interactions
- This type of approach began in the 50's, with early attempts to understand and model the nuclear force which led to the development of the first effective nuclear potentials (see, e.g., T.H.R. Skyrme, Nucl. Phys. 9, 615 (1959))
- The idea is to relegate the phenomenological input (i.e., parameters that need to be adjusted to data) to the effective interaction
- For nuclear properties calculated in a microscopic approach over the entire chart of the nuclei see, e.g., S. Hilaire and M. Girod's AMEDEE database:

http://www-phynu.cea.fr/science_en_ligne/carte_potentiels_microscopiques/carte_potentiel_nucleaire_eng.htm

- For properties of even-even nuclei in particular see, e.g., J.-P. Delaroche et al., Nucl. Phys. A771, 103 (2006)

The hierarchy of the microscopic approach

- Starting point is effective interaction between nucleons
  - Finite-range, fit a-priori, to very few nuclear data
- Simplest treatment of nucleon correlations is Mean Field
  - Valid if nearby excitations ≫ residual interaction (e.g., magic nuclei)
  - Otherwise true wave function mixes with nearby excitations
- Introduce correlations into Hamiltonian via successive improvements

1. $H_{true} \approx H_{MF}$ (Hartree-Fock)
2. $H_{true} \approx H_{MF} + V_{pair}$ (Hartree-Fock-Bogoliubov)
3. $H_{true} \approx H_{MF} + V_{pair} + V_{coll}$ (Generator-coordinate method)
4. $H_{true} \approx H_{MF} + V_{pair} + V_{coll} + V_{coll\text{-}intr}$ (GCM + qp excitations)
5. …

Tractable approach to a microscopic treatment of fission

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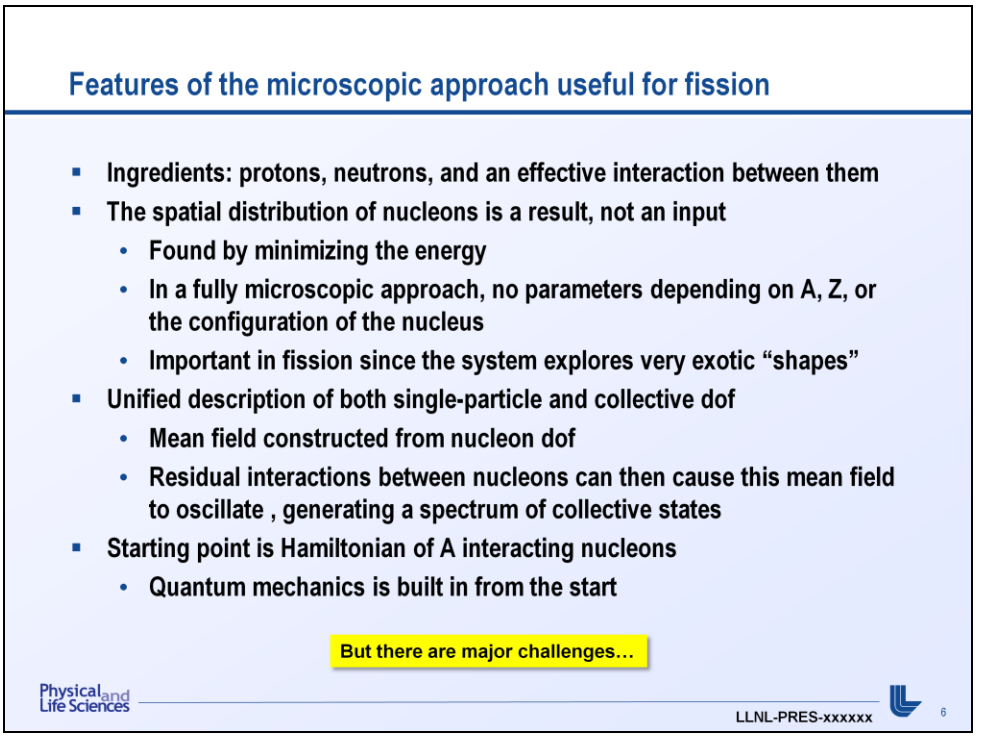
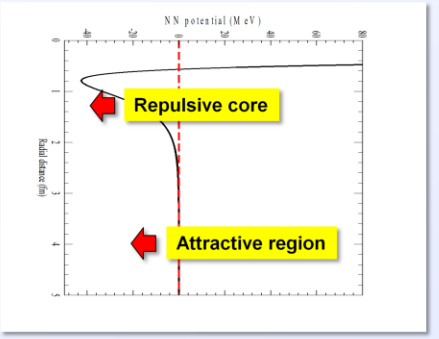
- One advantage of a microscopic approach is that the complexity of the quantum many-body problem can be treated in stages, through a hierarchy of successive improvements
- The starting point is the mean-field description, where the individual nucleons only feel an average potential, generated by the combination of all nucleons
- This pure mean field approach has been very successful in describing magic and near-magic nuclei
- The mean field is a coarse approximation, but it works well in magic nuclei because the residual interaction (the part of the nucleon interaction that is not account for in the mean-field approximation) is small compared to the energy of the first excited state. Thus, in magic nuclei, the mean-field approximation gives a reasonably good description of the ground state
- Far from magicity (as will be the case for fission, in general) it may no longer be the case that the residual interaction can be neglected compared to the excitation energy of low-lying states. In that case, quantum mechanics couples the ground and excited states, and the residual interaction can no longer be neglected
- Thus, we can follow a program of adding in the components of the residual interaction beyond the mean field in order of importance



- For the fission problem, such a microscopic approach is appealing for a variety of reasons
- The fissioning nucleus explores a variety of exotic "shapes" that cannot be directly probed by experimental measurements
- It also occurs in systems that are too short-lived to easily measure in the laboratory
- The parameters that enter into the microscopic approach (i.e., in the effective interaction) do not need to be readjusted for different nuclei, different shapes, or different energies of those nuclei. In particular, the same interaction can be used for the parent nucleus and its daughters
- Another appealing aspect of microscopic approaches is that collective motion (e.g., vibrations) are built up from the underlying single-particle degrees of freedom. In this way, the single-particle and collective motion are treated on an equal footing
- Furthermore, because the system is described by a Hamiltonian of interacting nucleons, quantum mechanics can be built in from the start
- But, of course, there are major challenges in implementing such a program

Challenge 1: we don't have a fundamental theory of the nucleon-nucleon interaction

We do not yet have a nuclear interaction completely derived from QCD



Although important progress is being made in that direction
(see, e.g., http://www.cenbg.in2p3.fr/heberge/EcoleJoliotCurie/coursannee/cours/D_lacroix.pdf)

For now, we use an effective interaction, with parameters adjusted to data

- The first challenge we must contend with is that, despite the fact that great strides are being taken in understanding the nucleon-nucleon interaction, we do not yet have a fundamental description of the nuclear interaction (i.e., derived entirely from QCD)
- The problem is that QCD is non-perturbative in the low-energy regime of nuclear physics
- In any case, whatever nucleon-nucleon interaction we could derive from QCD would be modified by complicated many-body effects inside the nucleus
- Thus, it makes more sense to use effective interaction, which are meant to capture the essential features of the bare interaction modified by the nuclear medium
- For an introductory overview of current trends in research into effective nucleon-nucleon interactions, see the course by D. Lacroix at http://www.cenbg.in2p3.fr/heberge/EcoleJoliotCurie/coursannee/cours/D_lacroix.pdf
- For a more in-depth discussion see, e.g., E. Epelbaum et al., Rev. Mod. Phys. 81, 1773 (2009)

Where do effective interactions come from?

- Realistic NN interactions cannot be used directly in many-body calculations because repulsive core prevents perturbative approach
- Brueckner & Goldstone devised a way to carry out the sums of infinite numbers of terms that account for the two-body interactions
- Inside the nuclear medium, Pauli exclusion limits the number of states that two nucleons can scatter into and prevents divergences due to the core
  - Thus the problematic bare interaction is replaced by a well-behaved "G matrix" describing the scattering of two nucleons inside the medium
  - The G matrix is the most important example of an effective interaction for the nucleus
  - Inside infinite nuclear matter, the Brueckner-Goldstone prescription can be calculated numerically and guides both the form and parameter values for the phenomenological effective interactions that are commonly used

- For an introduction to the Brueckner-Goldstone expansion technique, see B. D. Day, Reviews of Modern Physics 39, 719 (1967)
- See also M. de Llano, American Journal of Physics 38, 151 (1970) for a brief introduction to effective interactions
- For a discussion of the formal connection between the theory of infinite nuclear matter and one type of phenomenological interaction see J. W. Negele and D. Vautherin, Phys. Rev. C 5, 1472 (1972)

Effective interactions 101

- The N-N interaction is modified by its presence inside a nucleus
- Can be approximated by simple functional forms
  - Delta function ⇒ zero range — T.H.R. Skyrme, Phil. Mag. 1, 1043 (1956)

$$V(\vec{r}_1,\vec{r}_2) \sim \delta(\vec{r}_1-\vec{r}_2)$$

  - Gaussian ⇒ finite range — D. Gogny, in "Nuclear self-consistent fields", p. 333 (1975)

$$V(\vec{r}_1,\vec{r}_2) \sim e^{-(\vec{r}_1-\vec{r}_2)^2/\mu^2}$$

    - More computationally demanding than delta
    - Avoids mathematical pathologies of delta
    - This is what I will use for the rest of this lecture

For simplicity, I have not written all the terms.
There are a dozen free parameters from those terms

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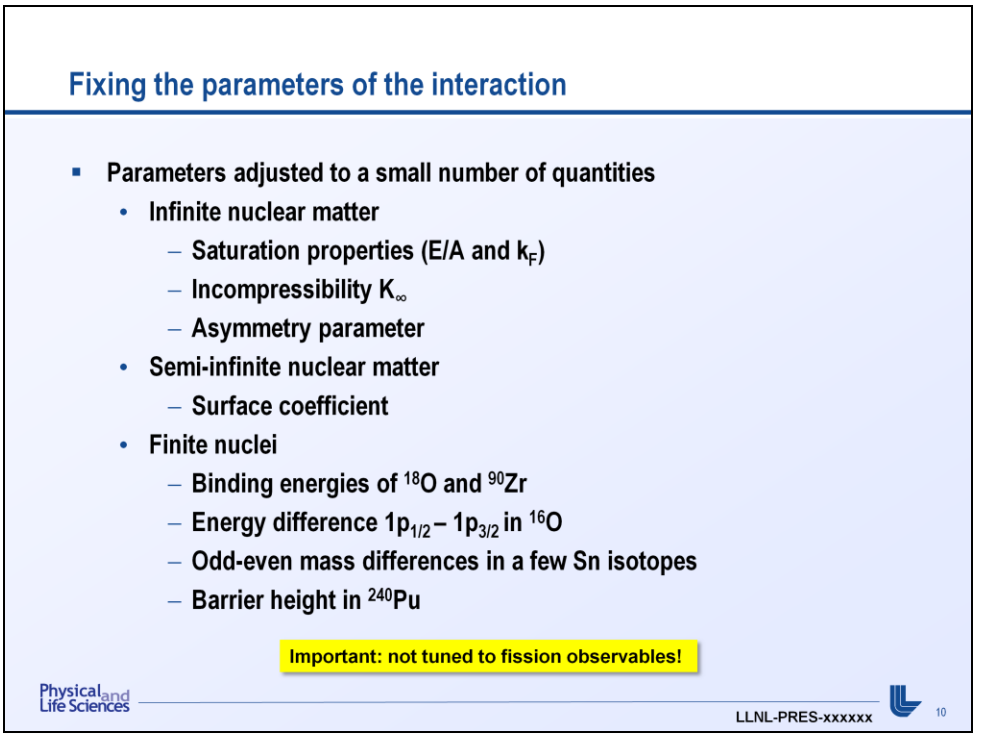
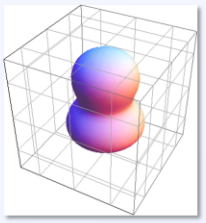
- Over the years, several functional forms have been used for these effective interactions
- One of the earliest, introduced by Skyrme, is the delta function
- The delta-function formulation has advantages (mathematical tractability) and disadvantages (pathologies due to infinities)
- Skyrme interaction are still widely used for a variety of applications in nuclear physics, including fission (see, e.g., J. McDonnell et al. in Proc. ICFN5, Sanibel Island FL (2012), p. 597, and references therein)
- In order to avoid the pathologies associated with the delta function, D. Gogny introduced a (finite-range) Gaussian form for the effective nucleon interaction. This is the form we will assume for the rest of this lecture



- Like any effective interaction, the finite-range interaction has parameters that must be adjusted to data
- In the traditional approach, those parameters are fitted to only a handful of nuclear data (namely properties of infinite and semi-infinite nuclear matter), and measured properties of a few finite nuclei
- More recent approaches have opted for a different strategy, fitting the parameters to a large number of experimental data (e.g. nuclear masses: S. Goriely et al., Phys. Rev. Lett. 102, 242501 (2009))
- For this talk, we will assume the traditional approach of fitting very few data that are not a-priori related to the fission observables of interest

Challenge 2: Fission is a difficult quantum many body problem



Sizing up the problem with a simplistic calculation:

For ^{240}Pu fission: distribute 94 protons & 146 neutrons on 3D spatial lattice + spin, 20 fm to the side, 1 fm spacing ⇒ $20^3 \times 2 = 16000$ lattice points:

$$\binom{16000}{94} \times \binom{16000}{146} \approx 10^{608} \text{ configurations!!!}$$

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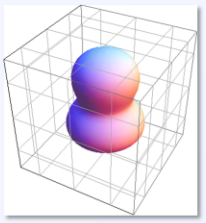
- The second difficulty we must face when we develop a microscopic theory of fission is the sheer complexity of the nuclear many-body problem
- We can illustrate the scope of the problem with a simple-minded, back-of-the-envelope calculation which, although not very rigorous nevertheless gives a sense of the difficulty involved
- Consider 240Pu as a fissioning nucleus, which has 94 protons and 146 neutrons
- Imagine this nucleus inside a cubic lattice 20 fm to the side (because that's a typical length for the fissioning nucleus) with lattice spacings of 1 fm (because that's roughly the range of the nuclear force)
- Allowing for spin, that's a total of 16000 lattice points. Now we wish to distribute the nucleons among those lattice points
- If we do not impose an a-priori picture of what fission "looks like", but instead we allow for all possible configurations that can arise from the scattering of nucleons into lattice points, the resulting number of possible configurations is beyond astronomical

Challenge 2: Fission is a difficult quantum many body problem



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- Too complicated to describe with full many-body wave function

⇒ Start with simplified picture, restore complexity in order of importance

⇒ Need High Performance Computing

⇒ Need to solve some tough conceptual problems

- What are the relevant degrees of freedom? (collective vs. intrinsic)
- How does the coupling between them affect fission?
- What is scission? How do we separate pre- and post-scission?
- …

- Thus, treating fission in a full many-body approach is hopeless
- And in fact, even if we could carry out such a program and obtain the full many-body wave function, those configurations corresponding to what we think of as fission would only represent an infinitesimal fraction of the full wave function. The remaining components would represent very exotic configurations that have nothing to do with fission (or indeed, may not even be found in Nature)
- Therefore, a better approach is to begin with a simplified picture that is directly relevant to fission (i.e., as a collective stretching of the nucleus), and add the complexity back in order of importance (remember the hierarchy of the microscopic approach we talked about a few slides back)
- Even with this simplified approach, there are still great challenges to overcome
- This still among the most (if not The most) computationally intensive problem in nuclear physics
- Quite apart from the technical/computational difficulties, there are also some complicated conceptual problems that have to be tackled having to do with quantum mechanics and its application to the nuclear many-body problem

The Hartree-Fock approximation

- The full many-body wave function has too many terms

$$\Psi = \sum_{\text{all configs}} c_{\text{config}} |\text{config}\rangle \qquad \text{number of terms} \sim \begin{pmatrix} \text{states} \\ \text{nucleons} \end{pmatrix}$$

- There are two commonly used solutions
  - The shell model: reduce the number of terms by restricting the number of states and nucleons to a few outside a closed shell
  - The Hartree-Fock approximation: replace Ψ with a simpler form:
    - Single Slater determinant, choose the one that minimizes the energy
    - e.g., for a system of 2 nucleons:

$$\Psi(\vec{r}_1,\vec{r}_2) = \frac{1}{\sqrt{2}}\begin{vmatrix} \varphi_a(\vec{r}_1) & \varphi_a(\vec{r}_2) \\ \varphi_b(\vec{r}_1) & \varphi_b(\vec{r}_2) \end{vmatrix} = \frac{1}{\sqrt{2}}\left[\varphi_a(\vec{r}_1)\varphi_b(\vec{r}_2) - \varphi_b(\vec{r}_1)\varphi_a(\vec{r}_2)\right]$$

This is not the most general form for Ψ(1,2,….): we are sacrificing some particle correlations for the sake of tractability

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- Once again: since the full many-body wave function is too complicated, we have to start from a simpler picture
- To put it in simple terms, the complication arises from the combinatorics of distributing many nucleons among many states
- Traditionally, there are two main approaches to build this simple picture:
- The shell model, which reduces the number of states and nucleons that have to be considered
- The Hartree-Fock approximation, which replaces the full many-body wave function and its enormous number of terms with a much simpler Slater determinant form
- Of course, this is an approximation, and the Slater determinant will never contain all the correlations of the full wave function
- Furthermore, in order to describe the lowest states of the fissioning nucleus, we must find Slater determinants that minimize the energy of the system (note that the Slater determinant that minimizes the energy is not unique, we will have more to say on this later in the lecture)
- Finding a Slater determinant that minimizes the energy is usually done through an iterative procedure that we will describe next

Solving the Hartree-Fock equations

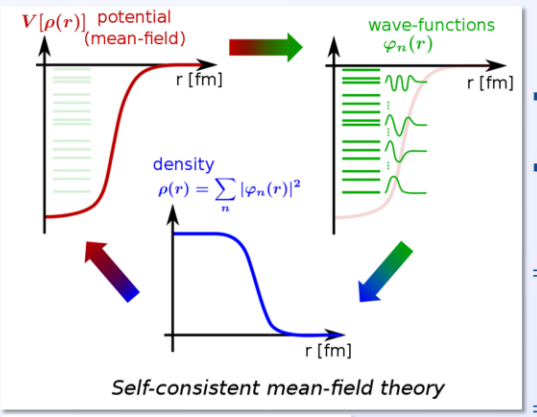


Image from commons.wikimedia.org

- From the Slater determinant, we calculate a one-particle density ρ
- From ρ we calculate a potential energy
- From the potential energy we get single-particle states $\varphi_n \Rightarrow$ Slater determinant

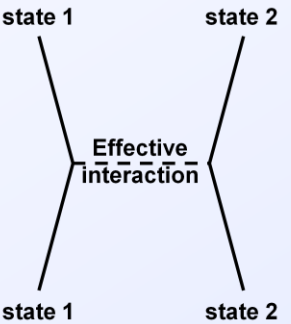
$\Rightarrow$ Hartree-Fock eqs are derived by a variational method and solved by an iterative process

$\Rightarrow$ Independent particles in a mean field, system in its lowest-energy state

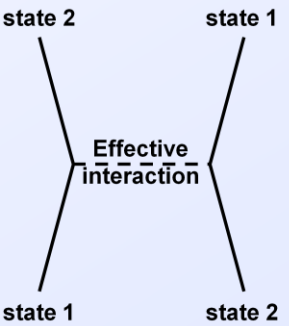
- If we start from an initial nuclear potential (that may be a guess), we can calculate single particle states in that potential
- We then construct a Slater determinant from those single-particle states and a corresponding particle density, rho
- By folding that density with the effective nucleon interaction, we can calculate the corresponding average nuclear potential, and once again obtain single-particle states from that potential
- And so on…
- At the end of this iterative process, we have a nuclear potential that has been obtained in a self-consistent manner (the nucleons generate the potential, and the potential determines the motion of the nucleons)
- The system of equations solved by this iterative process was obtained by minimizing the energy of the nucleus (in the Hartree-Fock approximation), therefore the solution in the end is the nucleus in its lowest energy state

Important aspects of the energy calculation

$$\text{mean-field energy} = \sum_{\text{state 1}} \sum_{\text{state 2}}$$

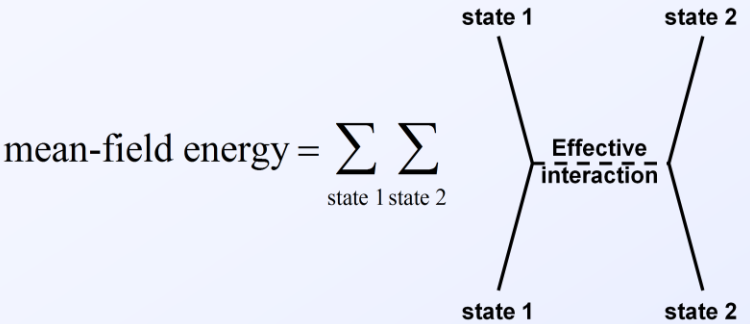


Also includes exchange terms:

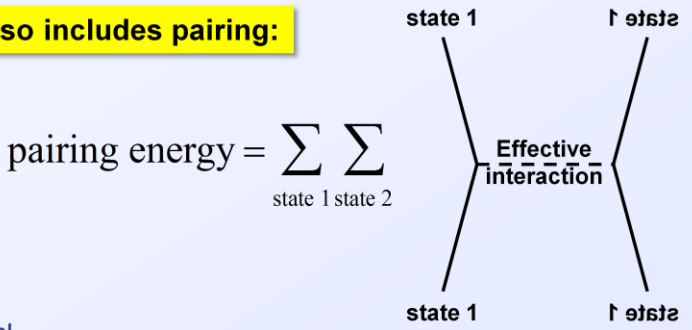


- The exchange term is present because of the anti-symmetrization of the overall wave function

Important aspects of the energy calculation



Also includes pairing:



Mean field and pairing involve different states, but the same effective interaction

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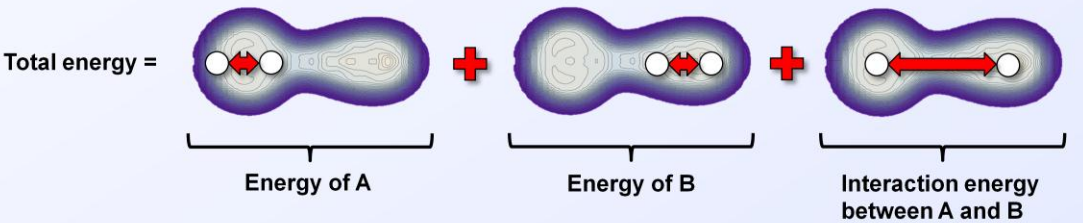
- As we mentioned before, the Hartree-Fock approximation works best in magic nuclei, where the residual interaction (beyond the mean field) is small compared to the energy of the first excited state
- For most nuclei, and for fission, this will not likely be a good approximation
- In particular, we know from experimental evidence that pairing plays an important role in the structure and properties of most nuclei
- In order to include pairing correlations, we must go beyond the Hartree-Fock approximation. This was done by M. Baranger, Phys. Rev. 122, 992 (1961), who generalized the Hartree-Fock method to "Hartree-Fock-Bogoliubov" in order to take pairing into account
- In the microscopic approach, no additional parameters are required to describe pairing; is arises from the sum of the effective interaction over correlated pairs of time-reversed states

Important aspects of the energy calculation

- The energy sum extends over all states in the nucleus
- But if you want to distinguish parts of that nucleus, you can always re-arrange the terms in the sum:



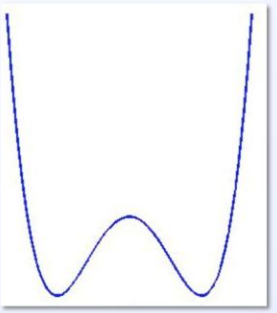
- The same effective interaction can be used to calculate the energy of
  - The whole
  - The parts
  - The interaction between the parts

This will be particularly useful when we discuss scission later on!

- If we wish to consider subsets of the nucleus, the terms in the sum can be re-grouped to reflect the contributions from the individual parts and their interactions
- This also means that the same effective interaction can be used for the parent nucleus from start to scission, and for the daughters
- And the same applies to pairing of course

Constrained Hartree Fock

Example:



- Two minima in potential
- How do we reach both minima with Hartree Fock?
- Add a constraint to the minimization process via the method of Lagrange multipliers:

$$\delta\left\langle \mathrm{HF}\left|\hat{H}-\lambda\hat{Q}\right|\mathrm{HF}\right\rangle = 0$$

In fact, with constraints we can explore the entire potential energy curve (and not just the minima)

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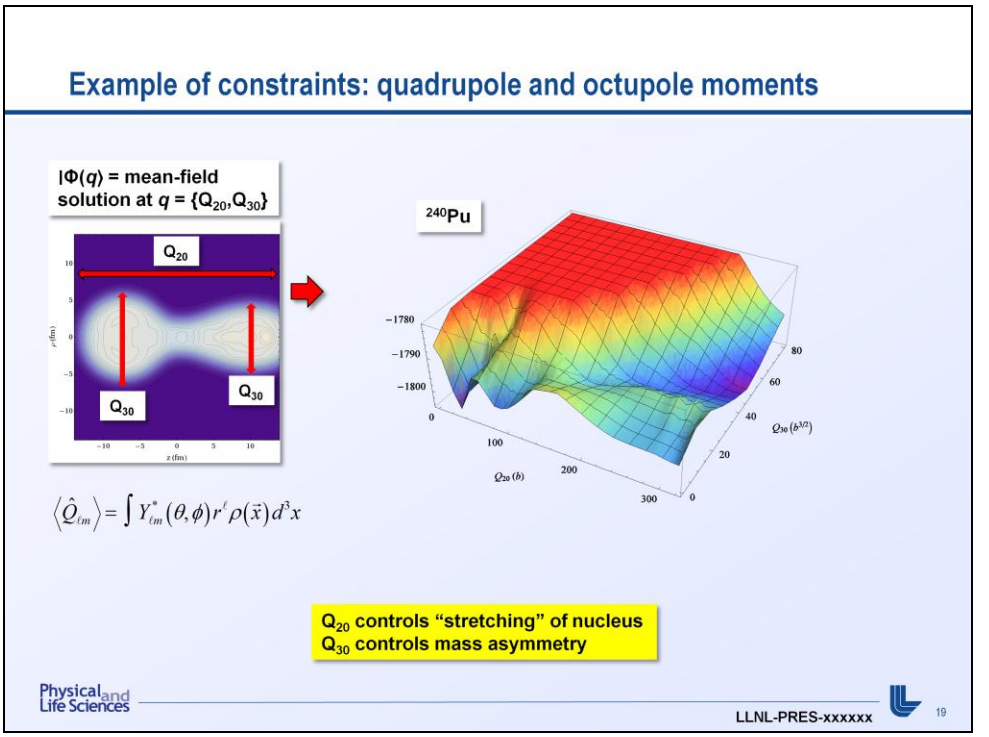
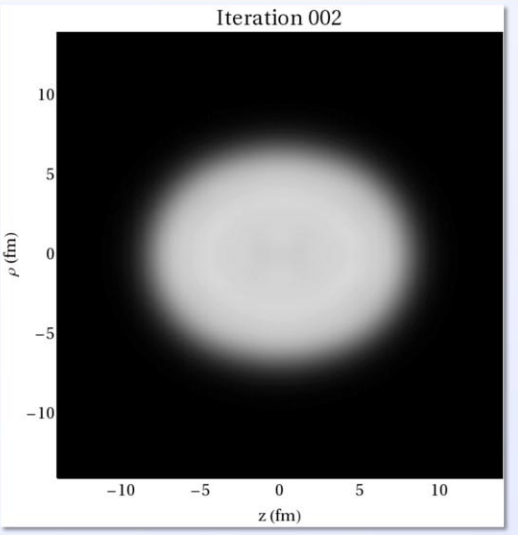
- So far the Hartree-Fock procedure we have described will always yield the state that is a (local) minimum in energy
- But what if we are in the situation shown above, with a two-minimum potential. Which solution will the Hartree-Fock procedure pick?
- The answer is that it depends on the starting point of the calculation (i.e., the initial potential or initial Slater determinant that the iterative process starts from)
- For fission, we will need not just some local minima but the entire potential energy surface
- In order to explore that surface, we can introduce constraints through the method of Lagrange multipliers

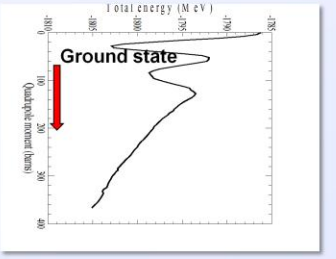


- Two commonly used constraints in the description of fission are the quadrupole and octupole moments of the fissioning nucleus
- The quadrupole moment (roughly) controls the elongation of the nucleus as it stretches toward its breaking points
- The octupole moment (roughly) controls the mass asymmetry of the nucleus, which eventually leads to its division into a light and heavy fragment

Example: ground state of ^{240}Pu



- Initial state = Slater determinant on deformed harmonic oscillator basis



- Density settles rapidly into ground-state configuration (variational methods love minima!)

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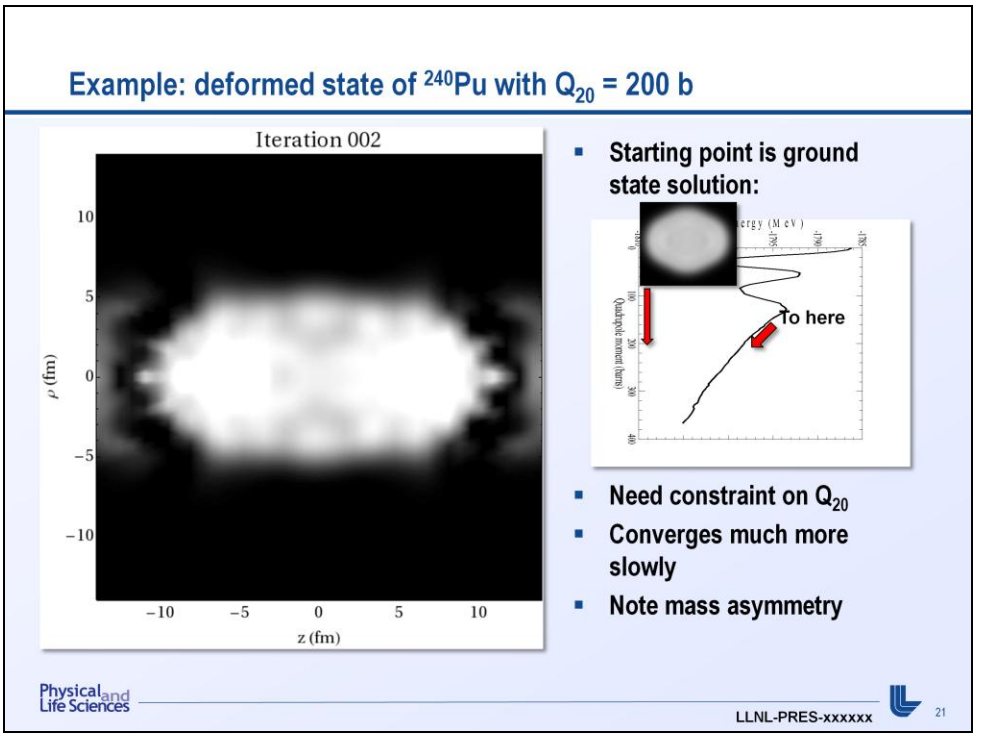
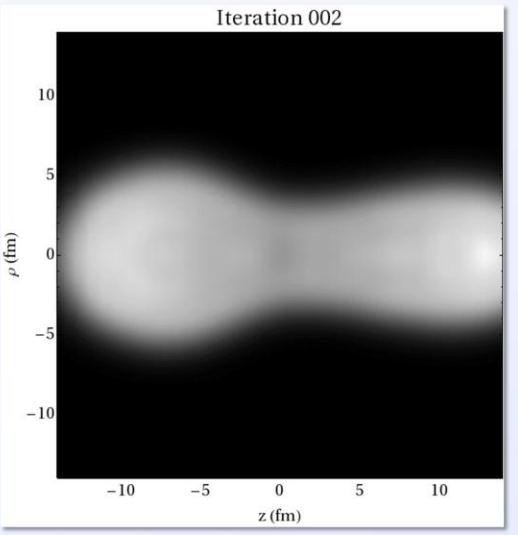
- Now let's look at some examples of HFB calculations
- First, we will try to recover the ground state of 240Pu
- In this case, I take as the starting point for the iterative HFB calculation a Slater determinant made up of deformed harmonic-oscillator states
- The animation shows the particle density in cylindrical coordinates of 240Pu over the course of the HFB iterations
- The density quickly relaxes into the ground-state configuration
- Note that this density is not homogenous: there is structure inside the nucleus

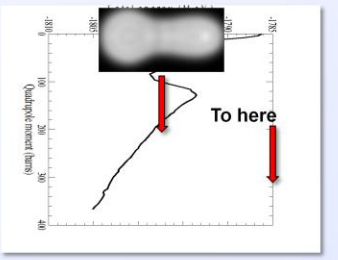


- Next, we look at a solution far from the ground state, with a quadrupole moment of 200 barns (compared to 28 for the ground state)
- Here, we need to introduce a constraint on Q20 to force the system to this deformation
- Normally such a calculation would be started from a nearby solution (e.g., one at Q20 = 196 barns), but in order to demonstrate the robustness of the convergence in the HFB iterations, we start from the ground-state solution obtained in the previous slide
- This time, more iterations are required, both because the starting point is far away, and because this solution is not at a stable minimum of the system
- Note the mass asymmetry of the nuclear "shape" at the end. HFB has broken the right-left symmetry that we began with, and we can start seeing a hint of what will become a light and a heavy fragment

Example: deformed state of ^{240}Pu with Q_{20} = 380 b



- Starting point is Q_{20} = 200 b solution:



- Need constraint on Q_{20}
- Converges very slowly
- Note that we have reached scission!

- Finally, let's stretch the nucleus to its breaking point by imposing the constraint Q20 = 380 b
- Starting from the solution in the previous slide with Q20 = 200 b, this time it takes over 400 iterations to reach a fully converged result
- But, in this way, we can explore all configurations relevant to fission; from the ground state, out to scission

Excitation mechanisms of the nucleus

Not a nucleus, but will do for now

Simplest: particle-hole excitation

More complex configurations can be built from a multitude of simpler particle-hole excitations

Collective motion in a "classical" movie:

then

then

then…

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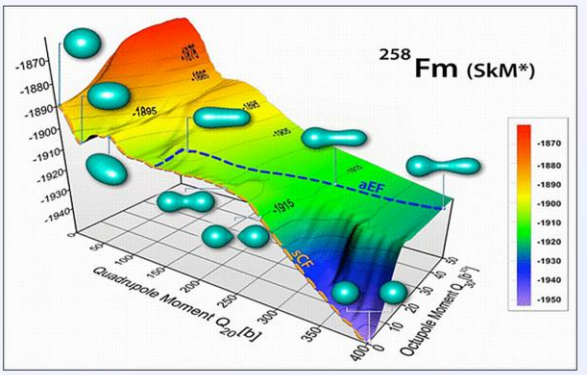
- We see examples of collective motion in systems, built up from the simpler motion of its constituents, at all scales in nature, for example:
- Murmuration of starlings (shown here)
- Flight of a swarm of bees
- Translational, rotational, vibrational, etc. motion can be decomposed into coherent sets of "single-particle excitations"
- In a classical picture, the different collective configurations can then be assembled into a sequence of frames which form a movie like the one shown here

The “quantum” movie of large-amplitude collective motion

- All frames for all possible flight paths and all possible configurations exist at the same time
- The “brightness” of each frame is what changes as a function of time
- All these frames, each with its own brightness, are shown at the same time

- In quantum mechanics, all configurations exist at the same time, but each has its own weight
- This is the principle of quantum superposition

Building collective motion from single particles: the nucleus



From ascr-discovery.science.doe.gov
Credit: *A. Staszczak et al., ORNL*

- Each point on map is a single-particle configuration: HFB ⇒ **Φ**(q)
- The nucleus explores many such configurations ⇒ form linear superposition of **Φ**(q):

$$|\Psi\rangle = \int dq\, f(q) |\Phi(q)\rangle$$

- Use variational procedure to determine the weights $f(q)$

- This is the Generator Coordinate Method (GCM) first proposed by Hill & Wheeler in Phys. Rev. 89, 1106 (1953)
- A truly quantum-mechanical description of collectivity built from single-particle degrees of freedom

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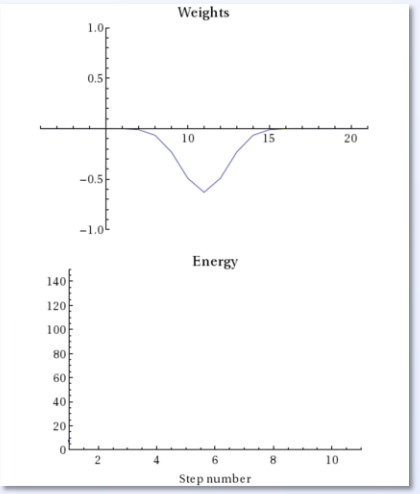
- If the difference in energy between states with different deformations is small compared to the residual interaction between quasiparticles, then (as we said earlier) the nucleus is "soft" with respect to the deformation and the states can mix
- In this case, no single HFB state gives a good representation of the ground state of the nucleus, and we must instead consider a mixture (or superposition) of states
- The weights of this linear superposition are the unknowns, and they are determined by a variational procedure that minimizes the energy of the nucleus with respect to this superposition of HFB states
- This approach, the GCM, was first proposed in the 50's by Hill and Wheeler
- The GCM goes beyond the mean-field approximation by eliminating the restriction to a single Slater determinant, and gives a truly quantum-mechanical description of large-amplitude collective motion in the nucleus. This is well-suited for the fission problem
- For an introduction to the GCM, see W. Greiner and J.A. Maruhn, Nuclear Models, Springer-Verlag (1996), pp. 346-353

Calculations using the GCM

GCM wave function: $|\Psi\rangle = \int dq\, f(q) |\Phi(q)\rangle$ &

Variational principle: $\delta E = \delta \dfrac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$



Numerical Example: harmonic oscillator

- Vary weights *f*(*q*) smoothly
- Look for stationary values in energy

⇒ Spectrum of collective states

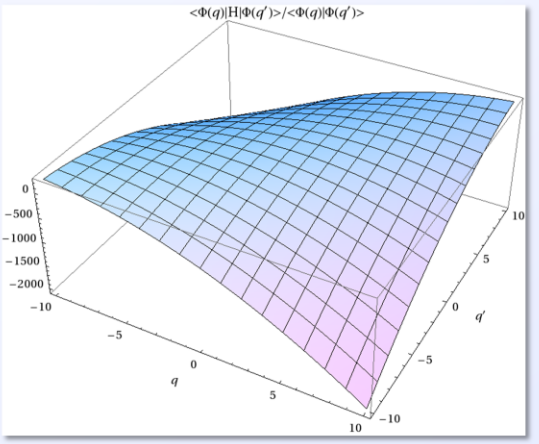
For more complicated H, this is not practical

- We illustrate the principle of the GCM with a simple example: the harmonic oscillator. This example is discussed in more detail on p. 348 of W. Greiner and J.A. Maruhn, Nuclear Models, Springer-Verlag (1996)
- In a variational approach, we would explore all possible values of the weights f(q) (and the complex conjugate f*(q)) independently to find stationary points in the energy functional, as illustrated here

Calculations using the GCM

GCM wave function: $|\Psi\rangle = \int dq\, f(q)|\Phi(q)\rangle$ **&** **Variational principle:** $\delta E = \delta \dfrac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle} = 0$

Let's look at the Hamiltonian overlaps for the harmonic-oscillator example:



And switch to coordinates:

$$\bar{q} \equiv \frac{q+q'}{2}$$
$$\delta q \equiv q - q'$$

- Applying the variational principle with this new, configuration-mixing wave function leads to the Hill-Wheeler (H-W) equation which involves integrals, derivatives, non-local and non-linear forms
- Note also that, in general, there is no reason to expect that HFB solutions at different deformations will be orthogonal, hence we are left with norm overlaps <**Ψ**|**Ψ**>
- In principle, the H-W equation could be solved numerically, but this is a tremendous technical challenge. In practice, the numerical solution of the full H-W equation has only been performed in cases with limited number of constraints q (see for example P.H. Heenen, in the Joliot-Curie school of 1991)
- We will take a different, more tractable approach here. Under certain conditions, the H-W equation can be brought into the form of a Schrodinger-like equation. The first step is a change of coordinates.

Calculations using the GCM

GCM wave function: $|\Psi\rangle = \int dq\, f(q) |\Phi(q)\rangle$ &

Variational principle: $\delta E = \delta \dfrac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} = 0$

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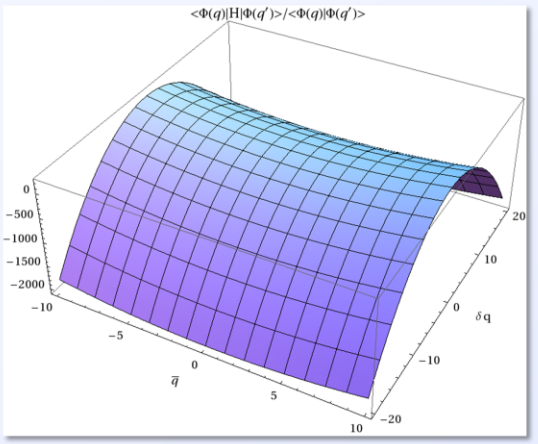


And switch to coordinates:

$$\bar{q} \equiv \frac{q + q'}{2}$$
$$\delta q \equiv q - q'$$

Expand overlaps to 2nd order in δq

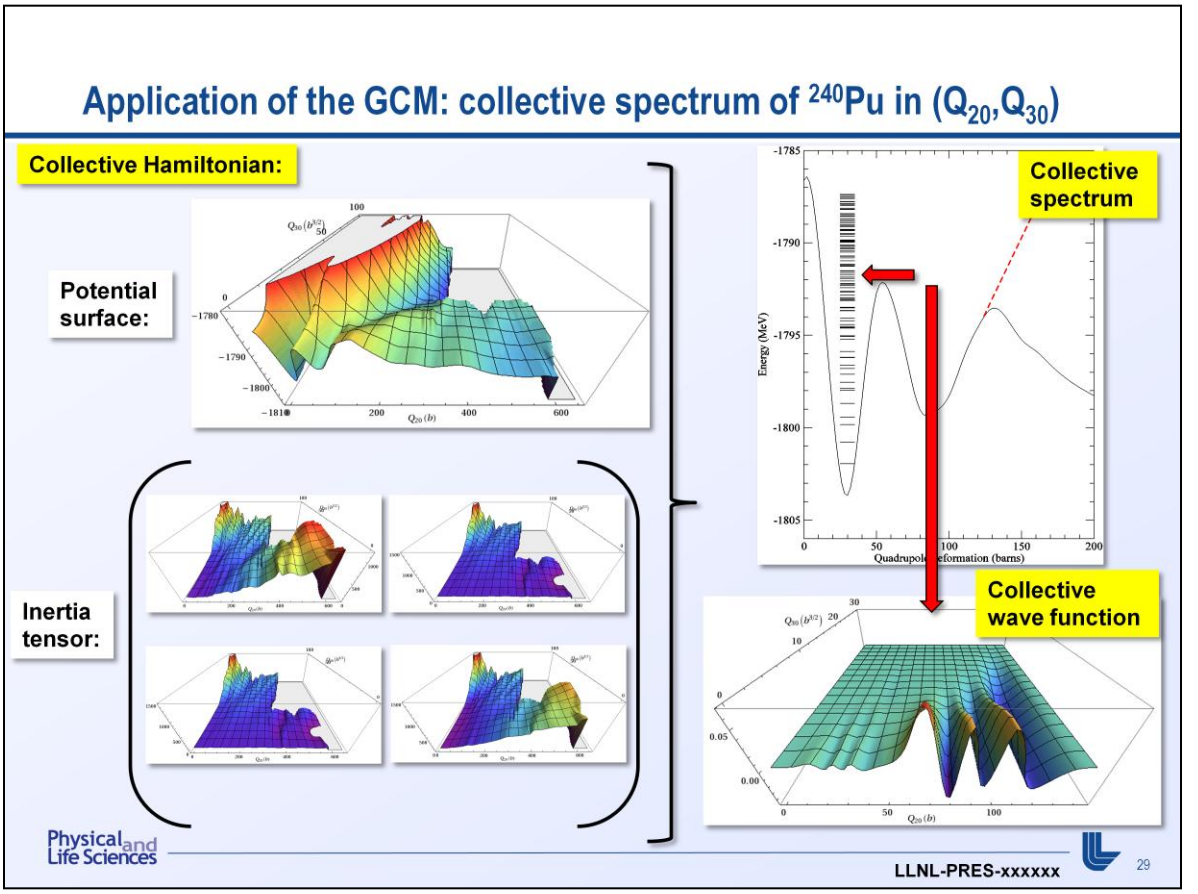
- For harmonic oscillator expansion is exact, otherwise it's an approximation

⇒ Schrodinger-like equation

⇒ Collective Hamiltonian

- In particular, curvature near $\delta q = 0$ is related to inertia of collective system

- In addition to making the calculations more tractable, recasting the H-W equation into a Schrodinger form yields a collective Hamiltonian constructed entirely from the underlying microscopic degrees of freedom. This microscopically derived collective Hamiltonian can be compared with those obtained in phenomenological approaches (e.g., the Bohr Hamiltonian)



- We show here a calculation of the collective Schrodinger equation for 240Pu
- On the left, the potential energy term is shown along with the components of the inertia tensor (since there are now two coordinates, these components introduce quadrupole-quadrupole, quadrupole-octupole, and octupole-octupole couplings)
- On the right, we show results of the solution of the collective Schrodinger equation
- At the top right we show the spectrum of collective states obtained. Note that the second barrier has been extrapolated to higher energies (dotted red line): this is done so that we can calculate quasi-stationary vibrational states localized in the first and second wells (see for example, O. Serot et al., Nucl. Phys. A569, 562 (1994) for further discussion)
- The bottom right panel shows the wave function for one of the collective states near the top of the barrier. Note how this wave function is localized in the second well.

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
  - From variational principle:

$$\delta \int_{t_1}^{t_2} dt \left\langle \Psi \left| \hbar i \frac{\partial}{\partial t} - H \right| \Psi \right\rangle = 0$$

With Ψ a Slater determinant

  - 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

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- According to the laws of QM, an initial state $|\mathbf{\Psi}(0)\rangle$ at t = 0 will evolve to a state $|\mathbf{\Psi}(t)\rangle = \exp(-iHt/\hbar)\,|\mathbf{\Psi}(0)\rangle$ where H is the full many-body Hamiltonian. In practice this is much too complicated
- The TDHF, originally proposed by P.A.M. Dirac (in Proc. Camb. Philos. Soc. 26, 376 (1930)), simplifies the problem by assuming the nucleus can be described by a Slater determinant at all times
- At any time t, the TDHF single-particle wave functions are not eigenstates of the Hamiltonian at that instant. Therefore the TDHF solution can describe excited states (with respect to the minimum energy state obtained by filling the lowest eigenstates of the Hamiltonian). In that sense, the TDHF does not have to be restricted by an adiabatic assumption
- Furthermore, the TDHF approach does not require a choice of collective coordinates: the equations of motion determine that path followed by the system
- Besides the technical challenges posed by the numerical solution of the TDHF equations, there are some conceptual drawbacks to the technique: 1) The restriction to a single Slater determinant leads to a description that is more classical in nature. 2) Tunneling is not permitted in the TDHF. The system follows a classical trajectory, conserving energy along the way. Thus if the initial density is inside a valley, the TDHF solution will remain in that valley for all times. 3) For a complex reaction where many final channels are open (e.g., fission), the single Slater determinant requirement introduces spurious cross-channel correlations that make it very challenging to describe these channels simultaneously (see, e.g., J.J. Griffin et al., Phys. Rev. C 21, 1351 (1980) and Y. Alhassid and S.E. Koonin, Phys. Rev. C 23, 1590 (1981))

Some developments in TDHF as a tool for fission

- 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 3-4 × 10^{-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)
- D. Lacroix, Phys. Rev. C 73, 044311 (2006): Stochastic TDHF: quantum jumps between Slater determinants
- I Stetcu et al., Phys. Rev. C 84, 051309 (2011): time-dependent density-functional theory

Could TDHF provide insight into the relevant degrees of freedom throughout the fission process?

- Despite the difficulties, the TDHF has been used to gain a deeper understanding of fission dynamics
- The advantages of the TDHF mentioned previously (e.g., non-adiabatic features, automatically determined fission path) make it an appealing tool for future research in fission
- For the purposes of this lecture, we will return instead to a time-dependent version of the GCM, which avoids many of the difficulties of the TDHF approach by not limiting the wave function to a single Slater determinant

Fission dynamics: the time-dependent GCM

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

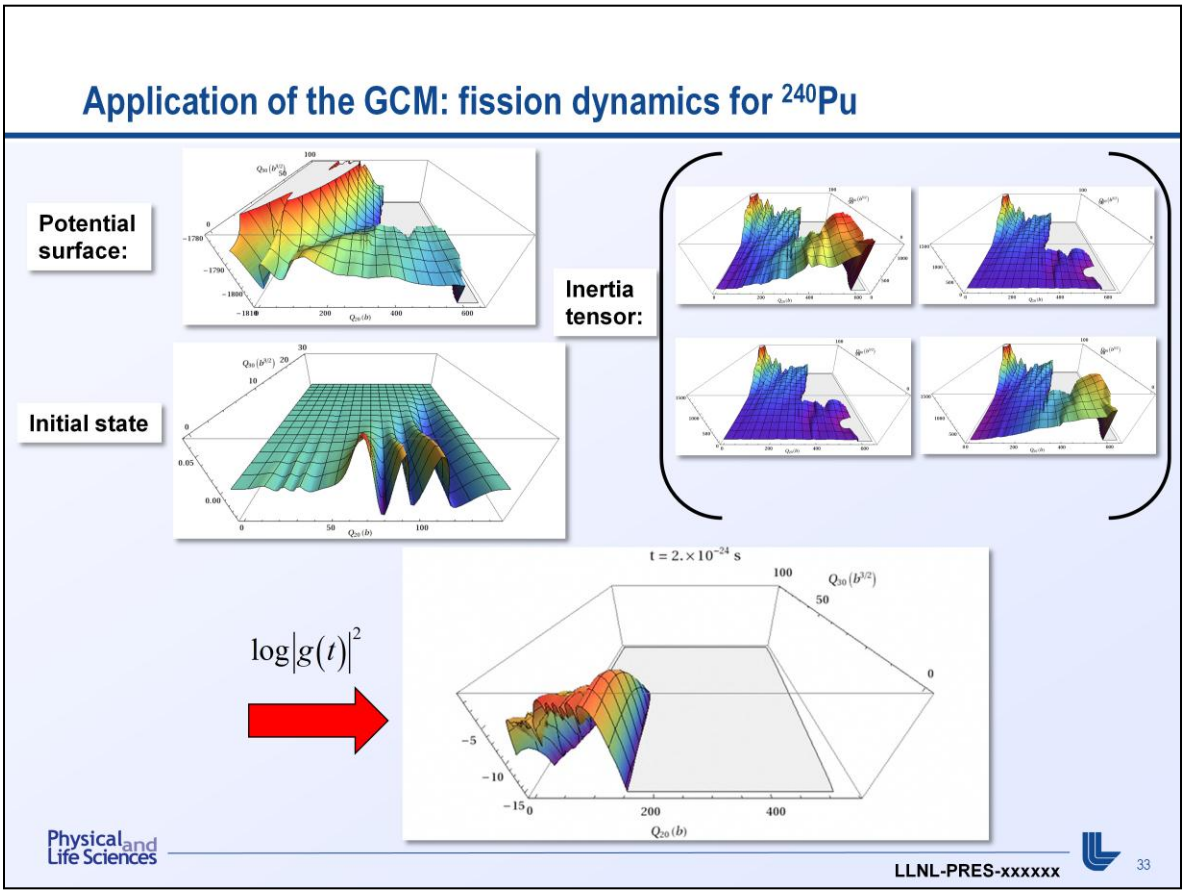
Variational principle + 2nd order expansion in non-locality

$$\delta \int_{t_1}^{t_2} dt \left\langle \Psi \left| \hbar i \frac{\partial}{\partial t} - H \right| \Psi \right\rangle = 0$$

With Ψ a superposition of Slater determinants (or HFB states)

- 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)

- The GCM ansatz can be generalized so that the weights include a time dependence. Applying the variational principle and expanding about the non-locality yields a time-dependent Schrodinger equation in the collective coordinates. In the process, we recover again the collective Hamiltonian that we obtained with the static GCM
- In order to solve this differential equation we need an initial condition, which is supplied by the collective states calculated in the static GCM a few slides back



- The same microscopic ingredients (energy surface, inertia tensor) as in the static GCM calculations enter into the calculation
- The result shown in the animation is a wave packet that evolves in time in the Q20-Q30 plane toward the scission configurations

Coupling between intrinsic and collective excitations in fission

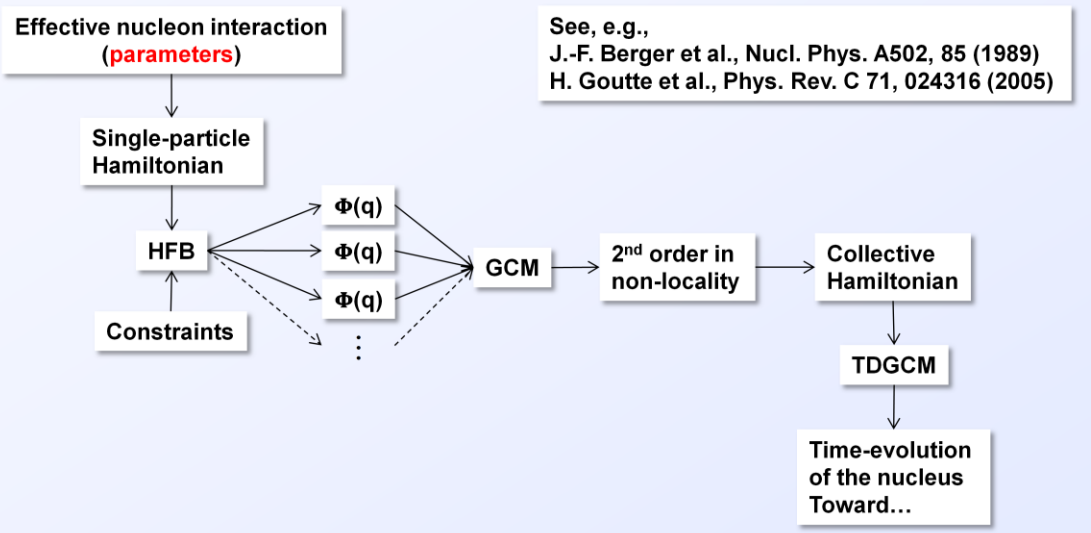
- **Develop GCM on a basis that includes intrinsic excitations**

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

- **Leads to generalized, non-adiabatic, Hill-Wheeler equation**
- **Can be reduced to Schrodinger-like equation**
  - **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)**

- So far, we have only considered collective modes in the fission calculations
- It is entirely possible that intrinsic (i.e., few quasiparticle) degrees of freedom can be excited as well during the fission process. These intrinsic excitations are not normally considered in microscopic fission calculations because of the technical complexity they introduce into the calculations
- From a conceptual point of view, the GCM can be readily extended to include such excitation with respect to the HFB minima. Following the usual procedure (variation, expansion about the non-locality) a generalized H-W equation is obtained that is no longer restricted to adiabatic conditions
- What is interpreted as dissipation in a semi-classical picture can now be described in a quantum-mechanical framework as coupling between collective and intrinsic degrees of freedom
- This type of approach is currently in development. See the work of R. Bernard et al. and references therein for further details

Recap: the microscopic approach so far



We're missing a crucial ingredient: scission

- So far, we have developed a consistent program to describe the fissioning nucleus from an initial state and throughout its subsequent evolution in time
- What is still missing is arguably the most important aspect of the fission problem: scission
- The question of how one quantum system becomes two is far from trivial, and we will tackle this problem next, in the second half of this lecture

A Microscopic Theory of Fission (part II)

FIESTA 2014 Summer School

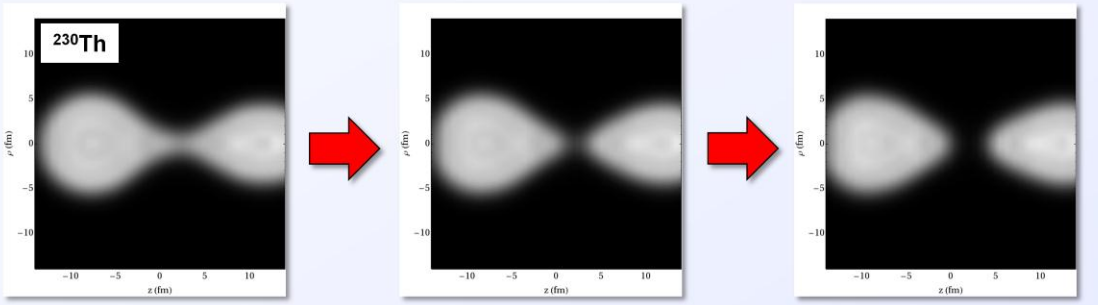
W. Younes

Physical and Life Sciences

Lawrence Livermore National Laboratory

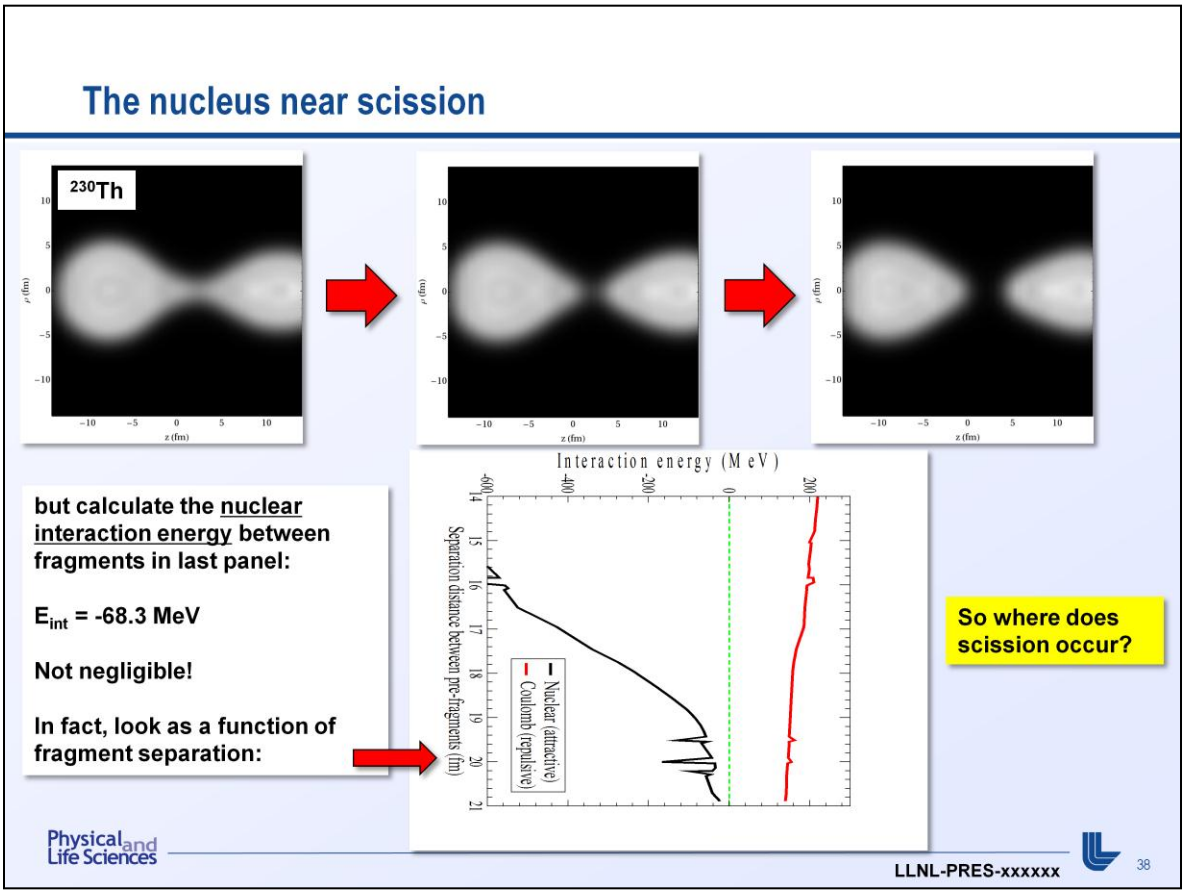
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Security, LLC, Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

The nucleus near scission



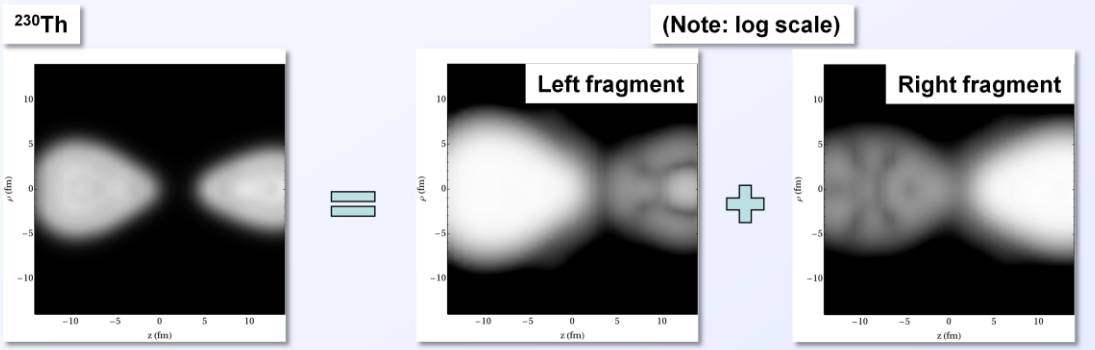
Microscopic calculation of the final stages of fission

- As a first step, let us consider scission from a geometrical perspective, by looking at the nucleon density in the final stages of fission
- Although there may be some question about the exact point at which scission occurs, there is clearly a “before” (first panel) and “after” (last panel)
- But in fact, this is an illusion…



- In quantum mechanics, geometric arguments based on the density can be misleading
- A better indicator of scission is the nuclear interaction energy between the two fragments. Since the nuclear force has a very short range (~ 1 fm), we expect this interaction energy to quickly vanish as the fragments move apart
- In a microscopic approach we can readily calculate this interaction energy without the need for any new ingredients, and we find that the energy is far from negligible (compared, e.g., to the separation energy of a nucleon, or ~ 6 MeV)
- In fact, this interaction energy never becomes negligible, even at relatively large separations between the fragments
- If this is truly the case, then scission never really occurs…

The nucleus near scission

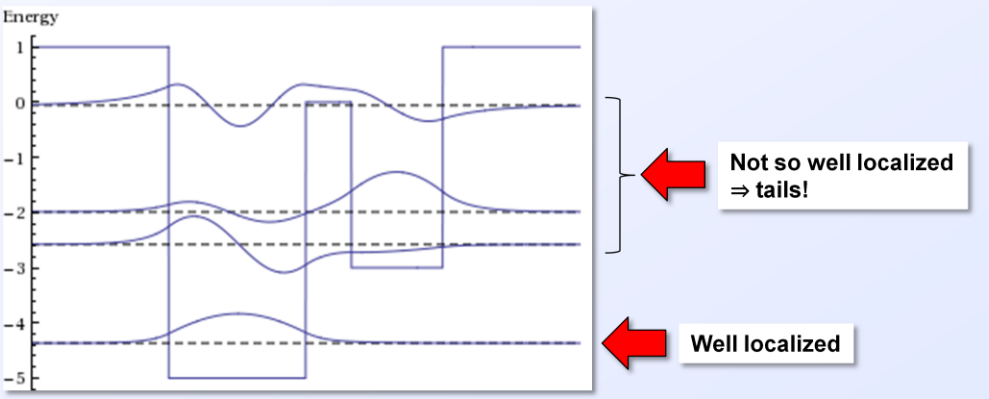


- The nucleon wave functions are delocalized, i.e., the fragments have tails!
- Tails are small but venture deep into complementary fragment!
  - Keep in mind: total nuclear energy of ^{230}Th in G.S. ~ -6.6 GeV
  - Each particle in tails contributes ~ -50 MeV to nuclear interaction between fragments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

- What is happening here is a beautiful manifestation of the non-local nature of quantum mechanics, and another example of the richness of the microscopic approaches
- We can get a better picture of what is going on by plotting separately the densities of the left and right fragments (to do this, we associate the single particle states whose wave functions are more localized on the left fragment with that fragment, and likewise for the right fragment).
- On a log scale, we see that these single-particle states are not completely localized on their respective fragment. Thus, each fragment has a tail extending into its complementary partner
- These tails may look small, but because they extend deeply into the heart of the complimentary fragments, they can give rise to very large nuclear energies. In fact, our calculations show that each particle in the tail contributes about an additional 50 MeV of binding energy between the fragments

The quantum localization problem in a simple model

- 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))

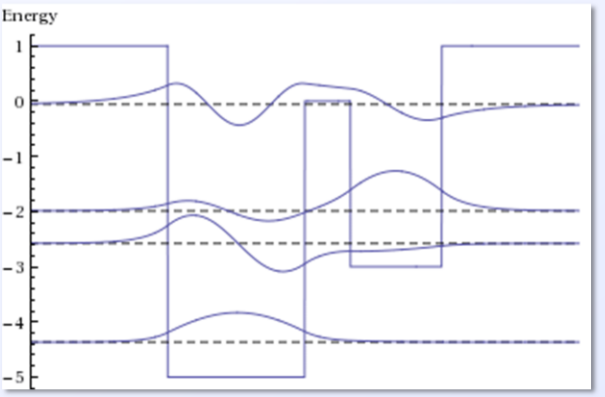


This is not a numerical issue, a basis problem, or a problem that is unique to nuclear fission: it is a direct consequence of the non-local nature of QM

- It is important to understand that this effect is not a consequence of any technical limitations in the calculations (e.g., numerical accuracy or basis choice)
- It is well known for example that the solution of the Schrodinger equation for a double-well potential in one dimension gives rise to delocalized orbitals. See for example the textbook by R. Gilmore.
- In this example, we use square wells so that the solution can be written exactly and explicitly in each region
- The question then is how do we define fission? And how do we recognize the pre-fragments progressively, as we approach fission, so that we may extract their properties at scission?
- In the microscopic approach I have described so far, this is the central point:
- We use wave functions throughout
- We want to recognize the pre-fragments on those wave functions

The quantum localization problem in a simple model

- 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))

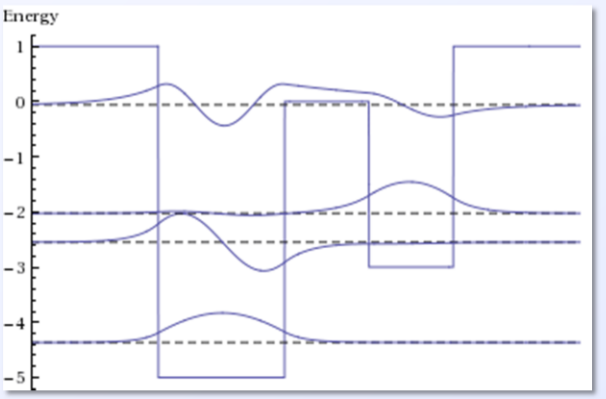


Moving the wells apart does seem to reduce the tails: problem solved?

- Here we simulate the pre-fragments moving apart before scission as the nucleus elongates by separating the 1D wells
- Note that the tails disappear!

The quantum localization problem in a simple model

- 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))



When accidental degeneracies occur, the tails come back!
This is what happens in the fission problem

- As the parent nucleus evolves toward scission however, the potential wells of the pre-fragments also change
- Here, we simulate this by making the well on the right progressively deeper
- As a consequence, single-particle levels move around, and can become degenerate in energy
- When a degeneracy occurs, the tails can reappear!

The concept of Localized Molecular Orbitals (LMOs)

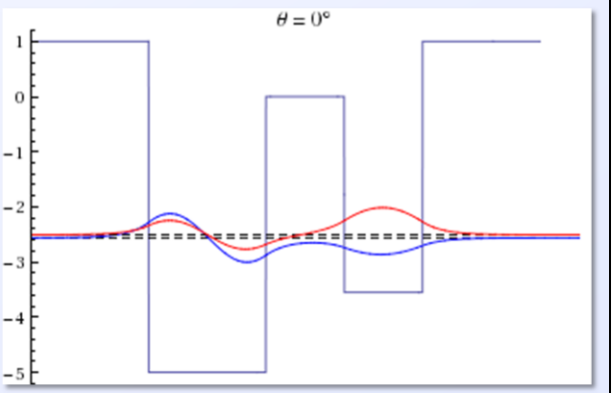
Sir John Lennard-Jones, Proc. Roy. Soc. A 198, 14 (1949):

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

Let's go back to our simple example and mix the two degenerate states with a rotation through angle θ



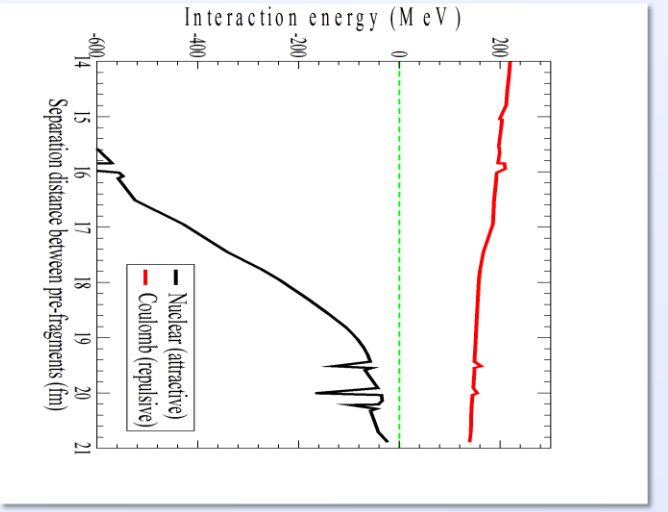
This is in the spirit of the "Localized Molecular Orbitals" used in molecular physics to construct physically meaningful orbitals (e.g., core, valence, bond) from delocalized Hartree-Fock solutions.

For fission: choose representation (i.e. transformation) that is appropriate to scission!

- The problem of delocalized orbitals is well-known in molecular physics.
- In addition, already in 1949, Sir Lennard-Jones had observed that orthogonal transformations of the components of a Slater determinant leave all the properties of the system unchanged
- Based on this observation, molecular physicists use orthogonal transformations to recast the delocalized electron orbitals produced in Hartree-Fock calculations into more physically meaningful states that can be identified with, e.g., valence, bond, core orbitals (see, e.g., Jan H. Jensen, "Molecular Modeling Basics" CRC Press (2010).)
- We can extend this concept to nuclear scission
- The HFB solution that is obtained by the usual variational procedure is not unique. In fact, any unitary transformation of this solution will produce another with the same energy, same values of the constraints, same global properties of the nucleus
- We illustrate this here using our simple 1D double-well example

The nucleus near scission: quantum localization

- **Remember: before quantum localization**

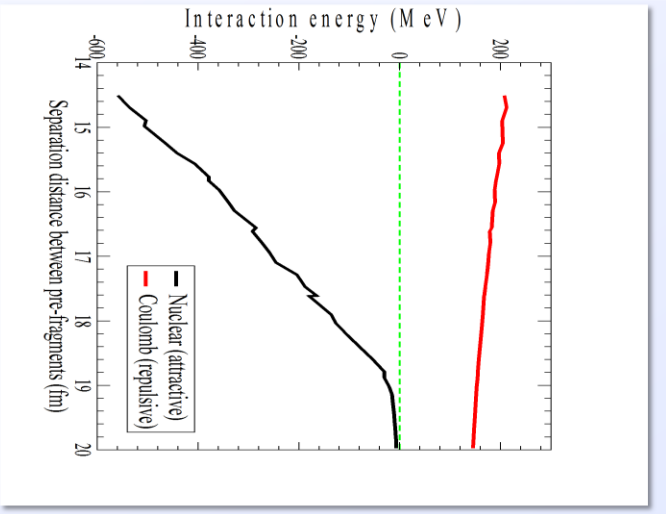


- We have already noted that the very large nuclear interaction energies between the fragments was caused by delocalized orbitals creating tails that extend into the complementary fragment

The nucleus near scission: quantum localization

- **Now: find a unitary transformation that reduces the tails**

⇒ **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!

- We have already noted that the very large nuclear interaction energies between the fragments was caused by delocalized orbitals creating tails that extend into the complementary fragment
- Therefore, if we find a unitary transformation that reduces the tails, this should reduce the nuclear interaction energy, and this is indeed the case
- We find that, with such a unitary transformation, we are now able to properly localize the orbitals on their respective pre-fragments before scission, and we can calculate an interaction energy between the pre-fragments that decreases as they move apart.
- With this procedure, we finally have a quantum-mechanical picture of scission

The quantum-mechanical definition of scission

1) **Coulomb force >> nuclear attraction between pre-frags (e.g., × 30)**

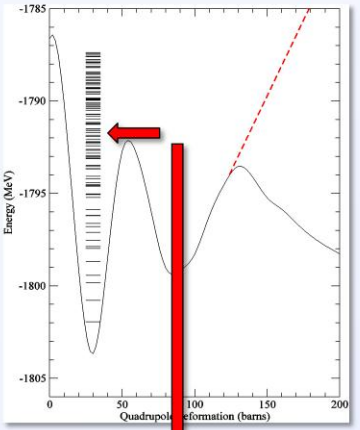
2) **Exchange interaction is small (e.g., < 1 MeV)**
   - ⇒ To good approx, can neglect antisymmetry between fragments
   - ⇒ $|\tilde{0}\rangle \approx |\tilde{0}\rangle_1 \times |\tilde{0}\rangle_2$ for all quantities of interest (energies, moments,...)

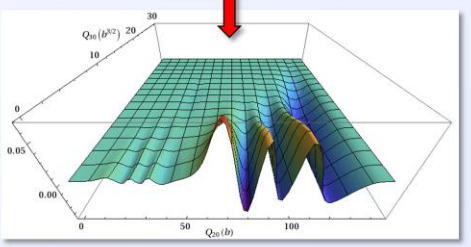
3) **Can excite local set of 2-qp states on each fragment**

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

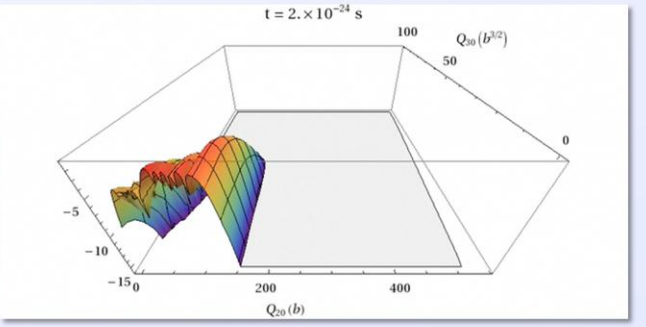
- We are now in a position to give scission criteria that incorporate the non-local aspects of quantum mechanics
- First, we expect at scission that the Coulomb force (which pushes the fragments apart) is much larger than the nuclear force (which tries to keep them together). This criterion is commonly used in other approaches, but in the microscopic approach, the forces are calculated in a consistent way from a single effective interaction between the fragments
- As a second criterion, we require that the exchange energy (which is a purely quantum-mechanical quantity) is small. This indicates that, to a good approximation, we can neglect the anti-symmetrization between fragments
- Finally, we should be able to generate quasiparticle excitation localized on each fragment. To put it another way, it should be possible to excite the individual fragments without destroying their localization
- With these criteria verified, we can truly treat the fragments as separate entities

Calculating fission yields





Recall the discussion of the TDGCM



We have a wave packet evolving toward the scission configurations

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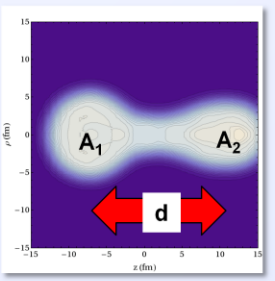
- Recall the earlier discussion of fission dynamics within the context of the time-dependent GCM
- We calculate a set of collective quasi-stationary states using the static GCM
- We then evolve those states in time, using the time-dependent GCM, toward the scission configurations
- Now that we are studying the wave packet as it nears the scission configurations, we need to revisit our original choice of collective variables to describe the fission process
- These calculations of fragment can be contrasted with those using other approaches, such as Brownian shape motion (Randrup & Möller, PRL 106, 132503 (2011)) and scission-point models (S. Panebianco et al., PRC 86, 064601 (2012))

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
- As the nucleus nears scission, local constraints (constraints on the individual pre-fragments) become important
- So, instead of Q_{20} and Q_{30}, we work with:

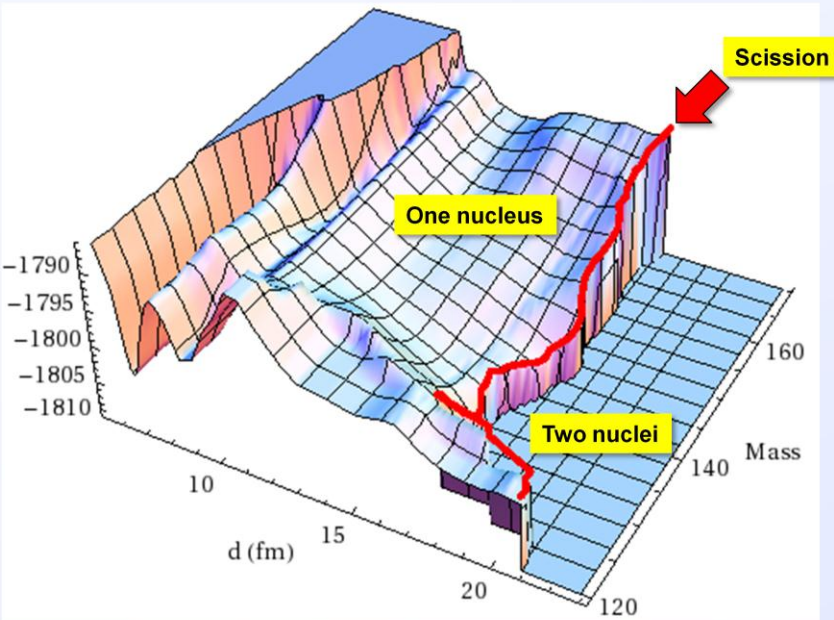
$$d \equiv z_2 - z_1$$

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



- Whereas multipole moments of the nucleus provide appropriate constraints for HFB calculation at low deformations (we know for example that, at these deformations, the nucleus exhibits low-lying quadrupole and octupole excitations), as we approach scission these are no longer necessarily the best constraints to describe the nucleus
- In fact, as we start to recognize pre-fragments within the wave function of the fissioning nucleus, it makes more sense to replace Q20 and Q30 with the separation distance between the centroids of those pre-fragments, and the actual number of particles in each pre-fragment
- In principle, we should use constraints calculated after the localization of orbitals previously discussed, in practice (and for the sake of computational simplicity) we use a semiclassical definition of these constraints before localization. However the subsequent analysis of the fragment properties at scission will be performed properly, after localization

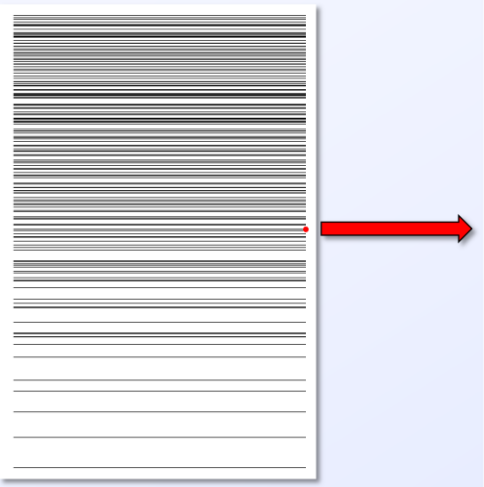
The scission line in the new coordinates



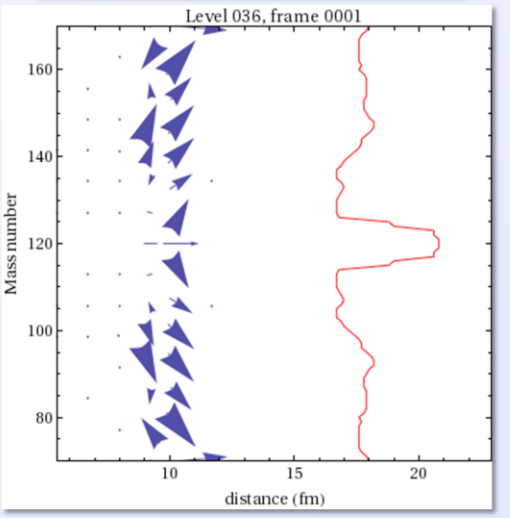
- The scission configurations form a line in the 2D plane defined by the new coordinates
- This scission line defines a boundary between a region where we have one nucleus (the parent), and two nuclei (the fragments)
- Note: with the new (d,A_H) (or, equivalently, (d,ξ)) coordinates, we have scission points for each mass division

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

^{240}Pu collective levels from GCM



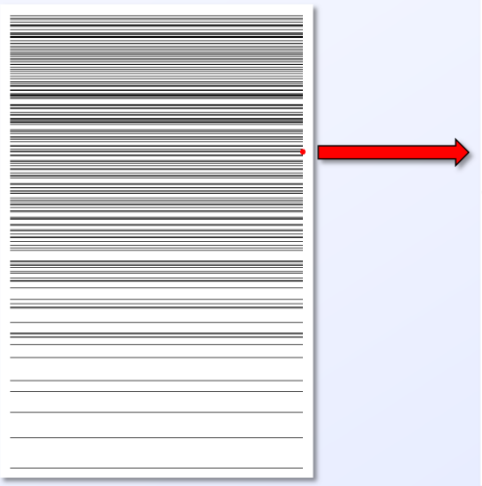
Time evolution of probability current



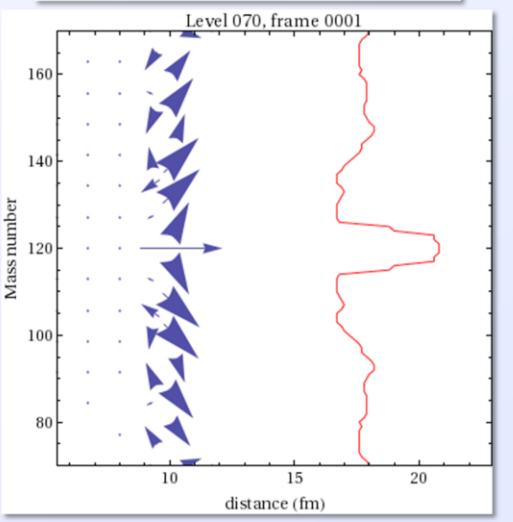
- Here we show the probability current for an initial state at low energy (corresponding to thermal fission)
- Note:
- very little flow for symmetric fission (A = 120)
- most of the flow is concentrated near most probable fission (A ~ 134 for heavy fragment and A ~ 106 for light fragment)
- the flow is fairly slow
- From this current, a flux can be calculated all along the scission line. We interpret this flux as a fission rate, and integrate it over time to get mass distributions for the fragments

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

^{240}Pu collective levels from GCM

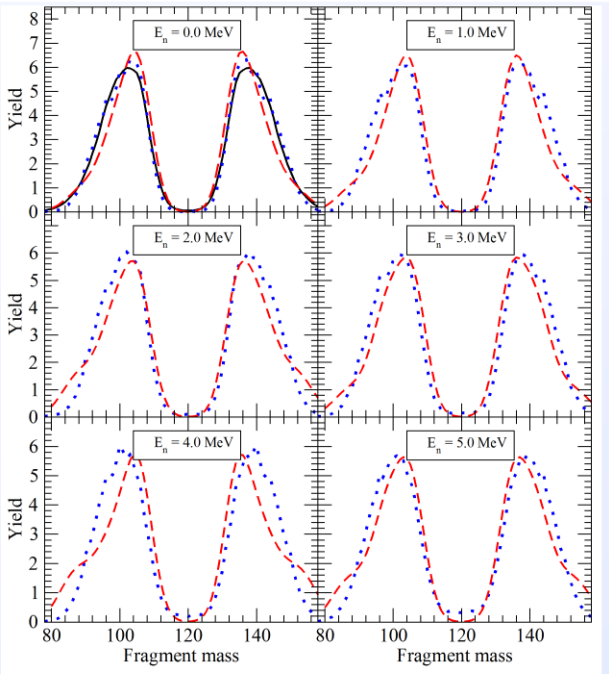


Time evolution of probability current



- This second example shows the current for an initial state at higher energy (by ~ 3 MeV)
- Note:
- a bit more flow in the symmetric case, but still not a lot
- more flow in the wings (A > 134)
- the flow dies down very quickly compared to the previous example

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

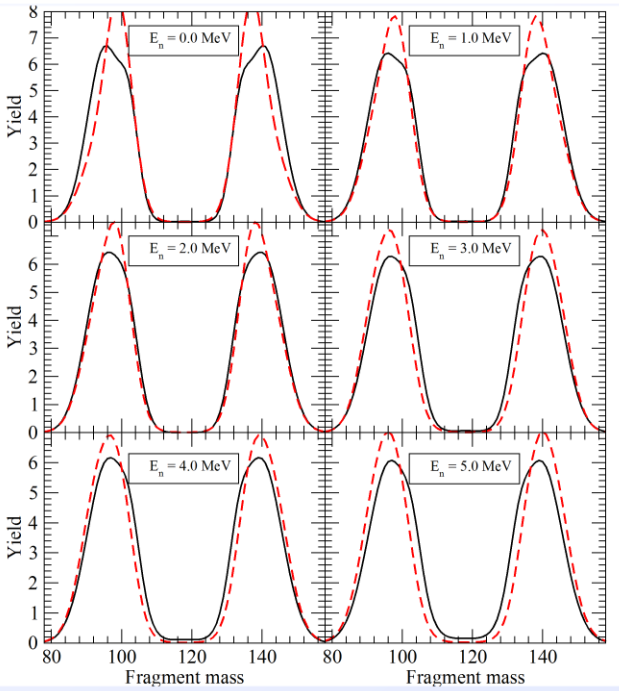


Microscopic calc
Schillebeeckx (92)
GEF code, Schmidt et al. (11)

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

- We show here similar calculations for n+^{239}Pu
- This time, pre-neutron emission yield data are only available for comparison at thermal energies (P. Schillebeeckx et al., Nucl. Phys. A545, 623 (1992)), for the remaining energies, we compare with calculations from the phenomenological GEF model (K.-H. Schmidt and B. Jurado, JEF/DOC 1423)
- Once again, these results are obtained starting from protons, neutrons, and an effective interaction between them

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



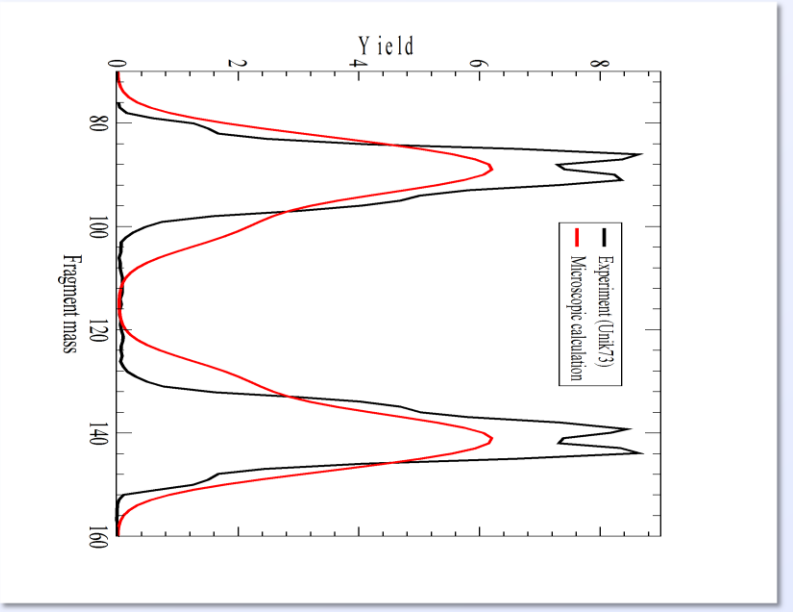
Microscopic calc

Straede (87)

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

- This is the same type of calculation, but this time for neutron on a ^{235}U target, and as a function of incident energy
- The different incident energies are obtained by starting from initial states at different excitation energies
- In this case the calculations are compared to the pre-neutron mass distributions measured by Ch. Straede et al., Nucl. Phys. A462, 85 (1987)
- Again, these results are obtained starting from protons, neutrons, and an effective interaction between them

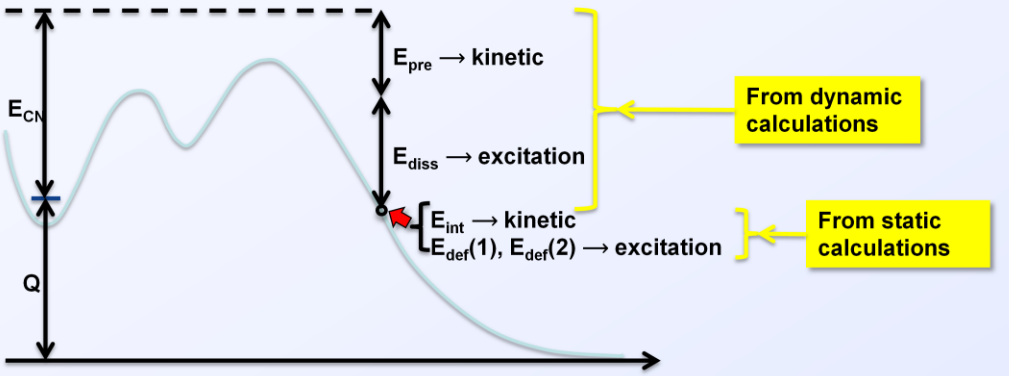
Pre-neutron fission yields for $^{229}Th(n_{th},f)$



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

- We show here an example of the mass yield calculated for thermal neutron-induced fission on ^{229}Th, obtained by integrating the flux across the scission line
- The calculation (red) is compared to experimental data from Unik et al., in Proc. Int. Symp. On physics and chemistry of fission, Rochester 1973 (IAEA, Vienna, 1973), vol II, p. 19
- Both experimental and calculated distributions represent yields before neutron emission
- It is worth remember that these results are obtained starting from protons, neutrons and an effective interaction between them

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)

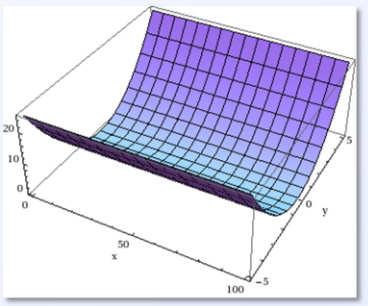
How do we partition the contribution from dynamics?

- Still within the framework of the same microscopic approach, we now turn to the calculation of the fragment (kinetic and excitation) energies
- There are two contributions to the energies of the fragments
- We can calculate a static contribution at scission, after localization. The HFB energy of each fragment calculated from its quasiparticle states at scission, minus that same energy when the fragment has been allowed to relax to its ground state without the complementary fragment present gives the excitation energy. The mutual Coulomb energy gives the static portion of the kinetic energy
- But there is also a contribution to both the kinetic and excitation energies of the fragments from the dynamic evolution of the system, this is the pre-scission energy we alluded to before
- We turn next to the estimate of this pre-scission energy
- This topic is of great importance for our understanding of the fission process, and has been explored using other approaches: see, e.g., W. J. Swiatecki and S. Bjørnholm, Phys. Rep. 4, 325 (1972), M. Mirea Phys. Rev. C 89, 034623 (2014)

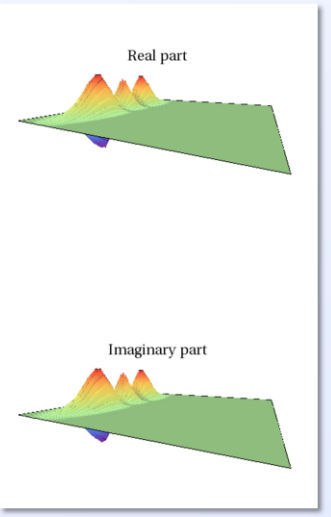
Pre-scission energy: a simplified example

Consider a potential surface
- **Flat in x direction**
- **Parabola in y dir**

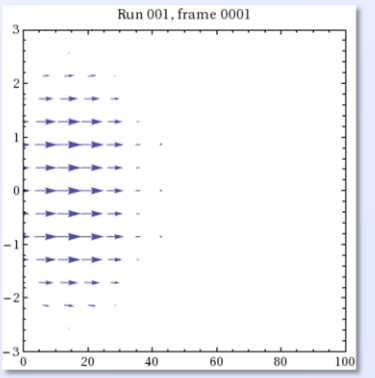
Inertia tensor
- **Large in x dir**
- **Small in y dir**
- **Zero in x-y**



And an initial wave function
- **Wave train in x dir**
- **Harmonic oscillator in y dir**



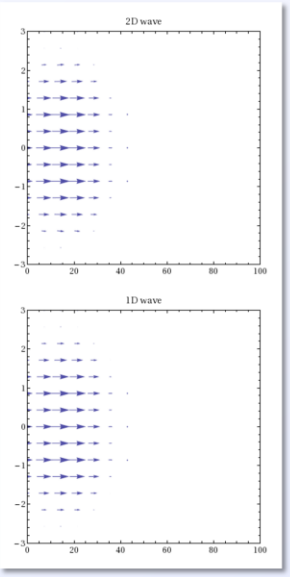
The probability current shows that the motion is not entirely in the x dir!



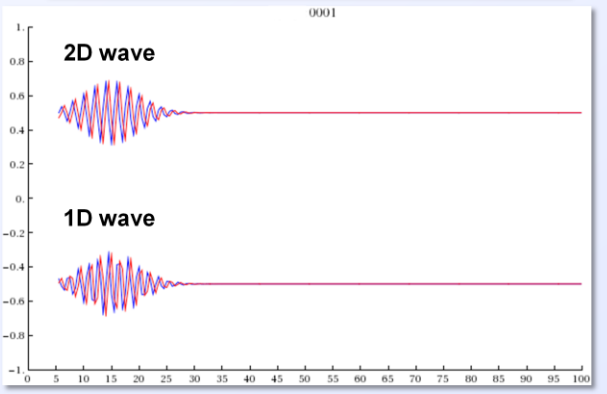
- We will illustrate the dynamical effects on the energy with this simple example, and using the collective Schrodinger equation derived from the GCM
- Note the transverse oscillations in the probability current
- not all the energy is in the direction of propagation
- we are interested in how the energy is partitioned between the two directions

Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir ⇒ 1D propagation in x dir



Notice also that the 1D wave is slightly faster:

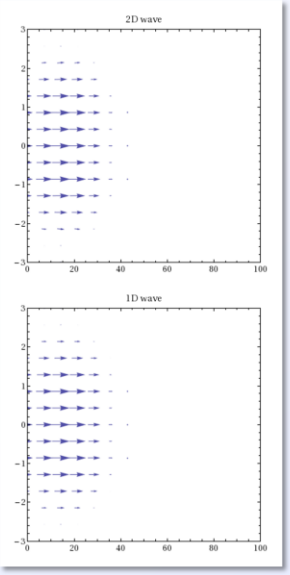


For fission, we can deduce the pre-scission kinetic energy from the energy difference between 1D and 2D, but how can we find this energy difference?

- To illustrate this further, we can repeat the calculation with the same initial wave packet, but this time eliminating anything that can give rise to motion in the transverse direction, i.e. we
- flatten out the potential surface
- set the component of the inertia tensor in the transverse direction to zero
- We refer to the resulting wave packet as the "1D wave" because it propagates essentially as if this were a one-dimensional problem
- The original (unmodified) wave packet is referred to as the "2D wave"
- By plotting a cross-sectional cut of the 2D and 1D waves (note that both the real (blue) and imaginary (red) parts of each wave are shown), we can see the effect of energy transfer to the transverse motion which slows down the 2D wave relative to the 1D one. The question is: by how much exactly?

Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir ⇒ 1D propagation in x dir



In this simple case, we know (by construction) that
- **For 2D wave: KEx = 4.97 (in arbitrary units)**
- **For 1D wave: KEx = 6.02 (in arbitrary units)**

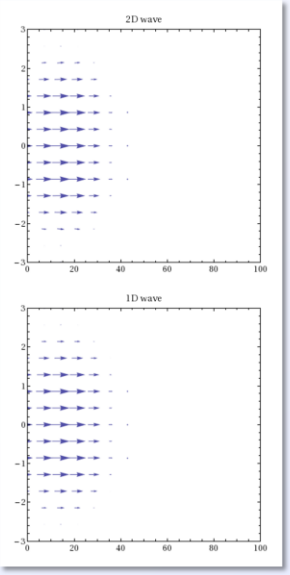
But in the realistic case, how do we find this?

One way is to sit at a point (e.g. x = 30, y = 0) and measure the flux in the x direction:
- **More flux ⇒ more kinetic energy**

- How can we quantify these observations?
- In principle, we could analyze the entire wave packet at each time step
- This becomes complicated when the wave packet is not a simple, well-localized function
- Instead, we will propose a method to extract the energy transferred to transverse motion from the analysis at a single point (which we will call an "exit point")

Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir ⇒ 1D propagation in x dir



In this simple case, we know (by construction) that
- **For 2D wave: KE_x = 4.97 (in arbitrary units)**
- **For 1D wave: KE_x = 6.02 (in arbitrary units)**

But in the realistic case, how do we find this?

One way is to sit at a point (e.g. x = 30, y = 0) and measure the flux in the x direction:
- **More flux ⇒ more kinetic energy**

We can even quantify this: if the 2D wave looks like a plane wave in the x direction then
1. **We calculate the normalized flux in x dir (flux divided by squared amplitude) at the measurement point**
2. **This normalized flux is constant in time**
3. **WKB gives the relation**

$$\frac{\text{normalized flux 2D}}{\text{normalized flux 1D}} = \sqrt{\frac{KE_x(2D)}{KE_x(1D)}}$$

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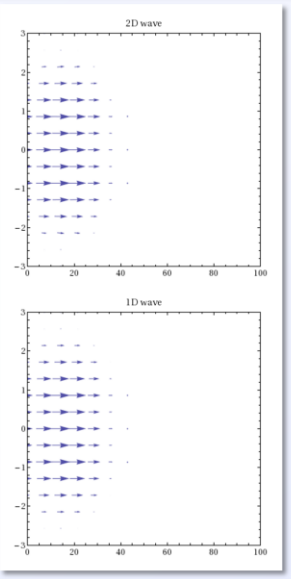
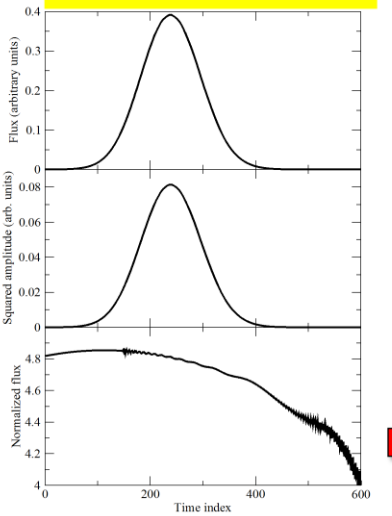
- To carry out this analysis, we use the WKB approximation, which lets us relate the normalized flux of a wave packet to its energy
- The important point here is that if we observe a wave packet solution from the time-dependent collective Schrodinger equation whose normalized flux is constant in time at an exit point, this behavior suggests a solution that is a plane wave in the direction of propagation, and some other function in the transverse direction. We never need to know this explicit form of the function in the transverse direction because it cancels out in the calculation of the normalized flux!

Pre-scission energy: a simplified example

Repeat with same initial form of the wave function with same total energy, inertia tensor nonzero only in x dir ⇒ 1D propagation in x dir



Normalized flux for 2D wave



We deduce: KE_x = 4.96

Compare to actual value = 4.97

- When we plot separately the flux in the direction of propagation and the squared amplitude at the exit point as a function of time, we find very similar behaviors for both: both rise to a maximum as the wave packet reaches them, and both fall away as it passes the exit point.
- The ratio of these two quantities (which gives the normalized flux) is relatively constant as long as a significant portion of the wave packet is passing through the exit point

Pre-scission energy: the more realistic case

- If we find a state with a normalized flux at a scission point that is constant in time, we can use the approach just described
- In fission calculations, the x coordinate will be the separation distance between pre-fragments
  - ⇒ We can identify KE_x with the kinetic energy of the pre-fragments at scission (i.e., the pre-scission energy)
- We invoke energy conservation to say that the remaining energy is transferred to collective modes of the pre-fragments
- These collective modes are not eigenstates of the final fragments
  - They will evolve in time as the fragments de-excite
  - That de-excitation energy will appear as neutron and γ emission

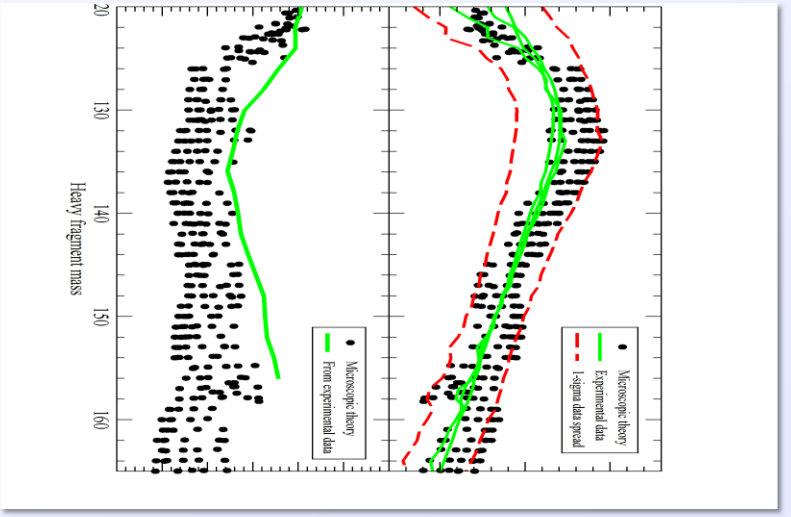
- We are still missing some physics: More collective & Intrinsic (quasiparticle) d.o.f.
- For now: excitation energy we calculate is a lower bound
- Calculations in (d,ξ) for most probable fission in $n_{th}+^{239}Pu$ is consistent with 50/50 split between kinetic and excitation from dynamic contribution

- We have described here a model to estimate the collective contribution to the pre-scission energy (for more details see W. Younes & D. Gogny, LLNL-TR-586694 (2012))
- Note that we are still missing contributions from additional collective and intrinsic d.o.f.
- As a result, the present calculations should be taken as a lower bound (but probably not too low)
- The microscopic calculations of fragment energies can be contrasted with the phenomenological models by Ruben et al. (Zeit. Phys. A 338, 67 (1991)) and Schmitt et al. (JEF/DOC 1423 (2011))

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

Calculated pre-scission energy due to collective coupling + expected additional few 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



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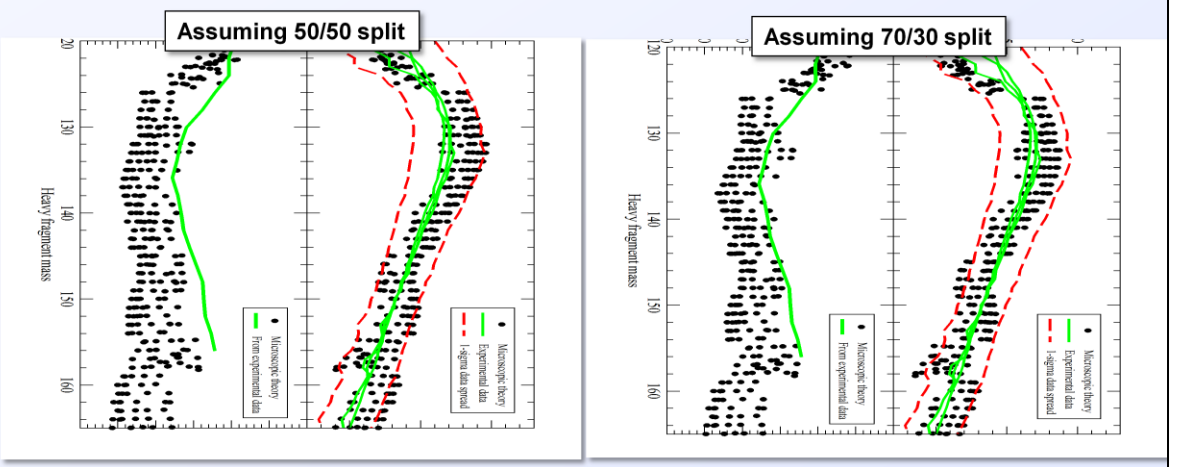
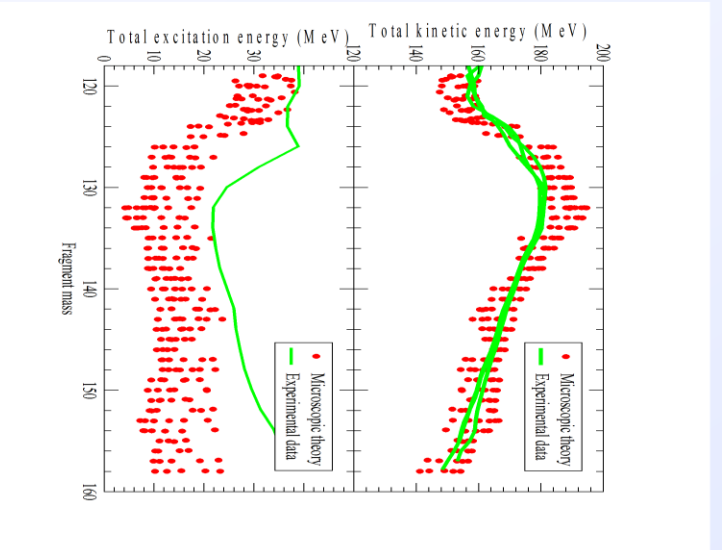
- For 239Pu(nth,f), the energy drop from saddle to scission for the most probable fission configuration is about 15 MeV
- We have calculated an 8 MeV contribution to the kinetic energy after coupling with one collective transverse mode. With additional coupling to intrinsic modes taking away a few more MeV, an assumption of 50/50 split of the pre-scission energy between kinetic and excitation energies seems reasonable.
- These quantities are consistent with other work using measured odd-even effects in fission products to deduce dissipation, see e.g. Gönnenwein in Proceedings Phys. And Chem. of fission, Zfk-646 (1988), p. 13.
- The resulting calculations of the total kinetic (TKE) and total excitation (TXE) energies are consistent with the data
- The TKE data shown here are taken from
- C. Wagemans et al., Phys. Rev. C 30, 218 (1984); K. Nishio et al., J. Nucl. Sci. Tech. 32, 404 (1995); C. Tsuchiya et al., J. Nucl. Sci. Tech. 37, 941 (2000)
- The TKE widths are from M. Asghar et al., Nucl. Phys. A311, 205 (1978)
- The TXE data are from J. Neiler et al., Phys. Rev. 149, 894 (1966)

TKE and TXE assuming different split of excitation/kinetic



- Even if more energy is dissipated into the excitation of the fragments through coupling with additional transverse modes, the results are still consistent with the data!

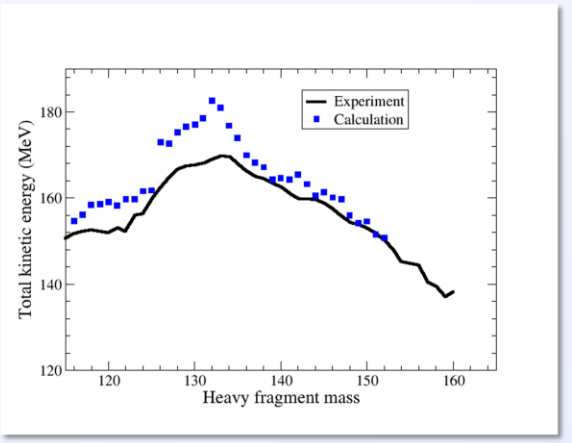
Results for $^{235}U(n_{th},f)$: fragment kinetic and excitation energies

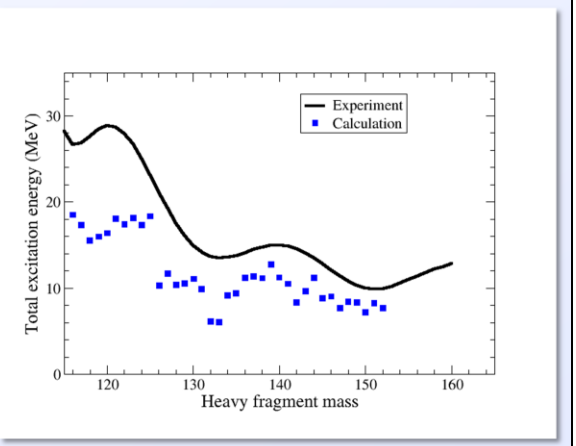


Starting from protons, neutrons, and effective interaction: Results consistent with experiment!

- A similar calculation for the thermal fission of 235U also gives reasonable agreement with the data
- All this was, once again obtained, without invoking extraneous models. Note in particular that we did not need to use statistical models or introduce a temperature to pump excitation energy into the fragments
- TKE experimental data are taken from: H. W. Schmitt et al., Phys. Rev. 141, 1146 (1966); P.P. Dyachenko et al., Phys. Lett. B 31, 122 (1970); H. Baba et al., J. Nucl. Sci. Tech. 34, 871 (1997)
- TXE experimental data are from H. W. Schmitt et al., Phys. Rev. 141, 1146 (1966)

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





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

- A similar calculation for the thermal fission of 229Th also gives reasonable agreement with the data
- All this was, once again obtained, without invoking extraneous models. Note in particular that we did not need to use statistical models or introduce a temperature to pump excitation energy into the fragments
- TKE data are from M. Asghar et al., Nucl. Phys. A373, 225 (1982)
- TXE data were obtained from Q values and TKE

Conclusions: summary

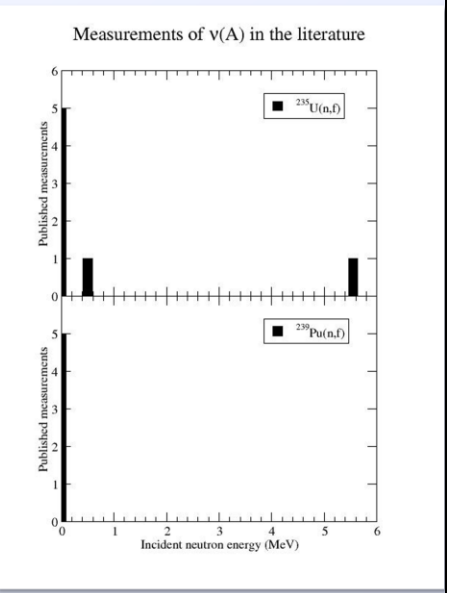
- Ongoing program to develop a microscopic theory of fission, starting from protons, neutrons, and an effective interaction between them
- Starting point is mean-field approximation, followed by a hierarchical restoration of correlations beyond the mean field
- Progress in understanding scission within 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 for theory

- Current effective interactions contain density-dependent terms
  - Need to move beyond this to fully non-local interactions
- What are the appropriate degrees of freedom throughout the fission process?
  - How do they evolve?
  - Can TDHF help?
- Calculate coupling between collective and intrinsic d.o.f., and its effect on fission observables
- Project wave functions to recover symmetries (e.g., angular momentum, particle number,…)

Experimental data needs

- **Need multi-parameter measurements, especially as a function of incident energy**
  - **Fragment yields & kinetic energies**
  - **Neutron energies & multiplicities**
  - **Gamma energies & multiplicities**
  - **⇒ Reconstruct nuclear state at scission**
- **Need measurements that directly probe fission dynamics**
  - **Scission neutrons**
  - **Fission times (with caveats)**
  - **Muon-induced fission**
  - **…**



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))

- In closing, we mention other work on various aspects of the fission process using microscopic approaches.
- This is by no means an exhaustive list, either in topic or in authors. It is only intended to show that there is extensive ongoing work on fission beyond what I have time to cover in this lecture

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))
- J. Erler et al., "Fission properties for r-process nuclei", Phys. Rev. C 85, 025 802 (2012)
- A. Staszczak et al., "Microscopic description of complex nuclear decay: Multimodal fission", Phys. Rev. C 80, 014309 (2009)
- H. Abusara et al., "Fission barriers in actinides in covariant density functional theory: the role of triaxiality", Phys. Rev. C 82, 044303 (2010)
- N. Dubray et al., "Structure properties of ^{226}Th and ^{256,258,260}Fm fission fragments: Mean-field analysis with the Gogny force", Phys. Rev. C77, 014310 (2008)

Useful reviews and books

- 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)
- E. Moya de Guerra, "The limits of the mean field", Lecture Notes in Physics 581, 155-194 (2001)
- W. Greiner and J. A. Maruhn, Nuclear Models, Springer (1996)
- J. A. Maruhn, P.-G. Reinhard, E. Suraud, Simple Models of Many-Fermion Systems, Springer (2010)
- P. Ring & P. Schuck, The Nuclear Many-Body Problem, Springer (1980)