Fission

Introduction to Nuclear Science

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The discovery and impact of fission

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The discovery and impact of fission

2 The fission process

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The discovery and impact of fission

- 2 The fission process
- 3 The way to scission



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- 3 The way to scission
- 4 The fissionability parameter



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- 5 The shell corrections



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- 6) The macroscopic-microscopic model

The discovery of fission

- Fission is discovered by chemists Otto Hanh and Fritz Strassman in 1938. The results are published in a German journal Naturwissenschaften (The Science of Nature).
- The series of experiments which led to the discovery of fission were intended in production of new elements heavier than Uranium through the neutron capture process on Uranium target.
- Chemical separation of the reaction products resulted in unexpectedly high yields of Lanthanum and Barium.
- This prompted the experimenters to a conclusion that Uranium split into fragments following the neutron capture.
- This conclusion had profound consequences for the history of mankind in the years to come.

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The impact of the discovery of fission

- Fission has been discovered in Nazi Germany shortly before the beginning of World War II in 1939.
- At the time of the fission discovery the Liquid Drop model developed by German scientists since 1935 has been relatively well established.
- The Liquid Drop Model allows to predict energy release from a fission of Uranium.
- The prediction is on the order of 200 MeV
- Typical chemical oxidation reactions, such as a TNT explosion, release energy on the order of a few eV (hundred million times less!).
- Potential for new type of weapon is quickly realized.
- Since the results are published the potential is realized at the same time by Germany, western allies, Soviet Union and Japan.

The chain reaction



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The impact of the discovery of fission

- Subsequent studies show that the fission fragments release neutrons.
- Thus the potential of self-sustained chain reactions and massive release of energy in an explosive way is realized.
- The race to construct nuclear weapons begins.
- In October 1939, prompted by a letter of Albert Einstein (Austrian) and Leo Shillard (Hungarian) US president F.D.Roosevelt initiates in collaboration with Great Britain and Canada the Manhattan project.
- The Manhattan project assembles western allies scientists and scientists who escaped Nazis expansion in Europe (many of them of Jewish origin) with a goal to construct nuclear weapon.
- The German project fails to produce a nuclear weapon, the same is true for the project in Japan.
- The Manhattan project succeeds and two nuclear bombs are dropped in August 1945 on Hiroshima and Nagasaki.

The impact of the discovery of fission

- Japan capitulates a few days after the Hiroshima and Nagasaki bombing.
- With the war in Europe concluded in May of 1945, the capitulation of Japan ends World War II.
- The nuclear race between western allies and the Soviet Union leads to the cold war which shapes the world politics until mid 1990.
- In parallel the process of peaceful utilization of nuclear energy is being developed.
- The nuclear technology (non-military as well as military) spreads out around the globe.
- The non-military effort leads to construction of nuclear power reactors for electric energy generation as well as research reactors for fundamental sciences, medicine and isotope harvesting.







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Image: A matrix and a matrix



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The way to scission

- How does a fissioning nucleus moves from the ground state to the saddle and scission point?
- To answer this question we should realize that the change of the shape is associated with a change of energy.
- The natural question is then what kind of energy?
- The answer is that there are two types of energies involved, the macroscopic energy related to the nuclear bulk properties as given by the liquid drop model and quantum mechanical energy associated with filling the shell model orbitals.
- In the simplest picture we can imagine this energy as forming barriers and wells in a deformation space describing the nuclear shape.
- A fissioning nucleus takes then the least energy path from the ground state to the saddle point subject to the conservation laws.

The way to scission



The liquid drop revisited

- In the dominant mode fission splits a single large nucleus into two fragments of comparable size.
- In the process, the Coulomb energy of the final system becomes reduced as protons become separated by a large distance.
- In the same process, however, the surface energy of the final system increases, as the surface area of the fragments is larger compared to the surface energy of the initial system.
- To investigate the interplay between the surface and the Coulomb energy let us turn into the Liquid Drop model.
- The fission studies become possible with the Liquid Drop model extension towards non-spherical, highly deformed, shapes.

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Liquid drop model's contribution



The Coulomb term

- Coulomb term accounts for electric repulsion between protons.
- An electrostatic energy contained within a uniformly-charged sphere of charge Ze and radius R can be calculated from the Coulomb law as

$$E_{Coulomb} = \frac{3}{5} \frac{1}{4\pi\varepsilon_0} \frac{Z^2 e^2}{R}$$
(1)

- The Coulomb law implicates the mathematical form of the Coulomb term: direct proportionality to Z^2 and inverse proportionality to $A^{\frac{1}{3}}$ (radius).
- The coefficient of the Coulomb term is fitted, it is negative as the term reduces binding.
- Coulomb term play a significant role for isotopes with large *Z* (actinides). With increasing *Z* it becomes larger than the volume term and limits the existence of stable isotopes.

Liquid drop model's contribution



The surface term

- Surface energy reduces binding.
- Surface term accounts for the fact that a nucleon at the surface of a nucleus interacts with fewer other nucleons than one in the interior of the nucleus and hence its binding energy is less.
- The magnitude of the surface term coefficient is negative and comparable in magnitude to the volume term.
- Surface term plays a significant role in light nuclei which have large surface compared to their volume. It accounts for the drop in binding energy at light masses.

Liquid Drop extension to deformed nuclei

- The Liquid Drop model which we discussed so far assumed spherical shape of a droplet of the nuclear liquid.
- This clearly can not work for fission, since we expect elongated shapes at the saddle deformation.
- The extension of the Liquid Drop can be studied using the expansion into deformed surfaces described by Legandre polynomials which are real number combination of spherical harmonics.

$$R(\theta) = R_0 \left(1 + \sqrt{\frac{5}{4\pi}} \beta_2 P_2(\cos \theta) + \sqrt{\frac{9}{4\pi}} \beta_4 P_4(\cos \theta) + ... \right)$$
 (2)

• Calculations should take care of conservation of nuclear volume.

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Deformed nuclear surfaces



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Fissionability parameter

Let us consider the lowest order expansion of the nuclear radius

$$\mathsf{R}(\theta) = \mathsf{R}_0 \left(1 + \alpha_2 \mathsf{P}_2(\cos \theta) \right) \quad \alpha_2 = \sqrt{\frac{5}{4\pi}} \beta_2 \tag{3}$$

Calculation of the Liquid Drop surface term yield

$$E_s = E_s^0 \left(1 + \frac{2}{5} \alpha_2^2 \right) \tag{4}$$

with E_s^0 being the surface energy for a spherical liquid drop.

• Calculation of the Liquid Drop Coulomb term yield

$$E_C = E_C^0 \left(1 - \frac{1}{5} \alpha_2^2 \right) \tag{5}$$

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with E_C^0 being the Coulomb energy for a spherical liquid drop.

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Fissionability parameter

With the above terms the deformed Liquid Drop energy becomes

$$E_{LD} = E_{LD}^{0} + \frac{1}{5}\alpha_{2}^{2}(2E_{s}^{0} - E_{C}^{0}) = E_{LD}^{0} + \alpha_{2}^{2}\frac{1}{5}(2E_{s}^{0} - E_{C}^{0})$$

$$E_{LD} = E_{LD}^{0} + \alpha_{2}^{2}\frac{2}{5}E_{s}^{0}(1 - x), \quad x = \frac{E_{C}^{0}}{2E_{S}^{0}}$$
(6)

- The above equation suggests that if x > 1 the Liquid Drop energy decreases with the increasing deformation parameter α₂; this leads to fission.
- The case of x < 1 implies that the Liquid Drop energy decreases with the decreasing deformation parameter α₂; this leads to spherical shapes.
- The parameter *x* is called the fissionability parameter.

The value of x

- The fissionability parameter is given by half of the ratio of the Coulomb to surface Liquid Drop energy.
- This is consistent with the earlier understanding of fission as resulting from the interplay between the Coulomb and the surface energy.
- The fissionability parameter can be calculated using the parameters of the Liquid Drop model

$$E_C^0 = a_C \frac{Z^2}{A^{1/3}}, \quad E_S^0 = a_S A^{2/3}, \quad x = \frac{a_C}{2a_S} \frac{Z^2}{A}$$
 (7)

• With the $a_S = 17.5$ MeV and $a_C = 0.7$

$$\frac{a_C}{2a_S} \approx \frac{1}{50} \tag{8}$$

The number of elements

- According to our model all nuclei with *x* > 1 fission.
- Thus the condition

$$x = \frac{1}{50} \frac{Z^2}{A} = \frac{1}{50} \frac{Z^2}{N+Z} = 1$$
(9)

set a limit on the highest Z which can be found in Nature.

For heavy nuclei the neutron to proton ratio is

$$\frac{N}{Z} = \frac{3}{2}$$
 thus $N = \frac{3}{2}Z$ (10)

Solving for Z

$$\frac{1}{50}\frac{Z^2}{\frac{3}{2}Z+Z} = 1 \implies Z = 125$$
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thus according to our model we should not expect elements beyond Z = 125.

• The largest Z element synthesized to date has Z = 118

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Limitation of the Liquid Drop model

- The Liquid Drop model is based on the bulk properties of nuclei, the volume, the surface, the atomic and the mass numbers.
- It is good to predict nuclear properties on average.
- The Liquid Drop model fails to predict the properties of specific individual nuclei, predominantly because it completely ignores quantum mechanics.
- It is apparent from a comparison of experimental and Liquid Drop binding energies per nucleon, which show significant deviations at the Shell Model shell gap closures.
- Thus the Liquid Drop model is useful in reproducing macroscopic (average) nuclear properties but not useful in reproducing microscopic (single nucleon) nuclear properties.

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Liquid drop model's mass fit



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The shell model

- Shell model is successful in reproducing microscopic, quantum mechanical properties of nuclei.
- In particular, it can reproduce shell gaps, energies, spins and parities of ground and excited nuclear states.
- Of significance to fission is the deformed shell model expandable to high deformation and exotic shapes which can appear on the way to the saddle point.
- We have discussed that nuclear deformation impacts shell ordering.
- Shell ordering, appearance and disappearance of the shell gaps play a crucial role in the fission mechanism as explained below.

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Axial, quadrupole-deformed harmonic oscillator in 3D

Note: without volume conservation, flat bottom or spin-orbit splitting.



Closed shell lowers the energy of the system



Open shell increases the energy of the system



The limitation of the Shell Model

- With all its successes, the nuclear Shell Model has a very profound deficiency, counting the energy of the occupied shells from the bottom to the Fermi level does not reproduce properly nuclear masses and binding energies.
- This results from the fact that the Shell Model is developed to reproduce properties of the orbitals near the Fermi level, but not these deep in the potential well.
- Orbitals near the Fermi level are crucial to reproduce nuclear properties which depend on the configuration of a few valence nucleons (spins, parities, excited states, reaction cross sections).
- The mass and binding energy depends on the properties of all nucleons, thus it is not well reproduced by the Shell Model.

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A successful marriage

- In summary, the Liquid Drop model deficiencies are not present in the Shell Model and the Shell Model deficiencies are not present in the Liquid Drop model.
- In 1967 a model which combined the strength of the Liquid Drop and the Shell Model has been proposed by Strutinsky.
- This approach separates the Shell Model energy calculated based on the occupation of orbits into a fast changing δE_{SM} part and the average part $\langle E_{SM} \rangle$.

$$E_{SM} = \langle E_{SM} \rangle + \delta E_{SM} \tag{12}$$

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 The average part is calculated by artificially assigning large widths to the states of the Shell Model.

A successful marriage

• The final energy assigned to the nucleus is equal to the sum of the energy of the Liquid Drop and the fast changing part from the Shell Model δE_{SM} which is called the shell correction.

$$E_{MM} = E_{LD} + \delta E_{SM} \tag{13}$$

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- This procedure effectively corresponds to the substitution of the Liquid Drop energy into the averaged energy from the Shell Model.
- This procedure is called the Microscopic-Macroscopic model or the Strutinsky shell correction model.
- It is very successful in calculating potential energy surfaces and barriers for nuclear systems.
- For examples see this link

The shell correction energy

