Chapter 1

INTRODUCTION

A scientist is not a person who has the right answers, but the one who asks the right questions.
- Claude Lévi-Strauss -

From the discovery of fission to fission barriers

Nuclear fission was first discovered by Hahn and Strassmann in 1939 and it immediately received much attention from both physicists and chemists alike since such a phenomena were unheard of at that time. Meitner and Frisch [1] coined the term fission to describe this phenomenon, whereby the nucleus is likened to a liquid drop which breaks into two smaller droplets. The existing semi-empirical mass formula (also known as the Bethe-Weizacker mass formula) was used to explain the fission process as a competition between the Coulomb repulsion and the surface tension of the nucleus. This idea was later on taken up and further developed by Bohr and Wheeler [2] for a more systematic description of fission. The liquid drop model was successful in describing the general trend of the nucleus as a function of deformation, i.e. the potential-energy landscape from the ground state up to the saddle point and then towards the scission point. Nevertheless, the model falls short of explaining many nuclear properties, for example why some nuclei have a deformed shape in their ground state, or the fact that the deformation energy of some heavy nuclei has a double peak. Improvement were later made by Strutinsky [3] in 1967 who proposed the incorporation of shell effects to the liquid drop model, giving rise to the microscopic-macroscopic model. In the 1970's, the theoretical study of nuclear structure takes on a new direction when calculations of global nuclear properties were performed from a microscopic view point via the Hartree-Fock (HF) method using an effective nucleon-nucleon interaction of the Skyrme type by Vautherin and Brink [4, 5]. This approach was then extended to large deformations by Flocard and collaborators using the constrained Hartree-Fock method [6] and was then applied to the study of the ^{240}Pu nucleus [7]. In recent years, many static calculations of the fission barriers have been performed microscopically based on the Skyrme [8, 9, 10], Gogny [11, 12, 13] and relativistic mean-field [14, 15, 16, 17] energy functionals. In all these approaches, one obtains the total binding energies as a function of nuclear deformations (deformation energy surfaces) from which the fission-barrier heights can be deduced.

Although fission-barrier heights are not observable quantities, they are still important for many reasons. From a nuclear reaction point of view, the fission-barrier heights play an important role in determining whether the excited compound nucleus deexcites through neutron evaporation or fission. In order to facilitate the occurence of fission, the information on the fission-barrier height can assists in determining the amount of excitation energy needed in the compound nucleus for fission to occur by adjusting the energy of the incident projectile. On the other hand, fission barriers are an input for the calculations of fission cross-sections whereby the latter are directly comparable to the experimental data. In cases when the intended compound nucleus is hard to produce from nuclear reactions, the fission cross-sections for this nucleus can be predicted using fission barriers obtained from theoretical predictions.

From a different point of view, the fission barriers play a role in describing the stability of a nucleus from spontaneous fission. The stability of a nucleus with respect to spontaneous fission is related to its fission half-life, the calculation of which involves fission barriers. With recent technological advances, more and more exotic superheavy nuclei are being produced. For such unstable nuclei, the probability for fission increases and fission becomes an important decay mode to achieve nuclear stability in competition with α decay. In this case, a reliable estimate of the fission-barrier heights is all the more important [1] due to the short-lived nature of these nuclei.

In view of the wide application of fission barriers in nuclear reactions and nuclear energy as well as the understanding of spontaneuous fission, it is therefore important to improve on the theoretical approaches from which the fission barriers are obtained. While many fission-barrier calculations have been performed for even-mass (with even numbers of protons and neutrons) nuclei, there are comparatively very few microscopic studies dedicated to odd-mass nuclei. The main reason is the complication caused by the breaking of time-reversal symmetry at the mean-field level for a nuclear system composed of odd numbers of nucleons (fermions).

Mean-field calculations of fission barriers of odd-mass nuclei

One of the earlier microscopic study of odd-mass actinides at large deformation was performed by Libert and collaborators in Ref. [18] for the band-head energy spectra in the fission-isomeric well of ^{239}Pu within the rotor-plus-quasi-particle approach. More recently, fission-barrier calculations were performed within the Hartree-Fock-Bogoliubov approach by Goriely and collaborators [19] for nuclei between between $88 \leqslant Z \leqslant 96$ (Z here referring to the atomic number). The resulting fission barriers were then used

[1] As was pointed out in Ref. [29], a variation of 1 MeV in the fission-barrier heights will translate into a change of approximately four order of magnitudes in the fission half-life.

for the neutron-induced fission cross-section calculations as part of the RIPL-3 project published in Ref. [20]. At around the same time, Robledo and collaborators have performed fission-barrier calculations of ^{235}U nucleus [21] and ^{239}Pu nucleus [22] within the equal-filling approximation (EFA) presented in Ref. [23]. In practice, the EFA allows one to "break" the odd-nucleon (unpaired) into half and place one half in a specific single-particle states and the other half in the time-reversed state. In this way, the time-reversal symmetry is not broken and the calculations are performed as in the ground state of an even-even nucleus. However, in the Bohr and Mottelson picture the total angular momentum (total spin) of the odd-mass nucleus corresponds to the projection of the total angular momentum on the nuclear symmetry axis K of the blocked single-particle state, i.e. $I = K$.

Although the EFA was found to be a good approximation [24], a proper microscopic description of odd-mass nuclei requires the consideration of all the effects brought upon by the unpaired nucleon. This nucleon gives rise to non-vanishing time-odd densities entering the mean-field Hamiltonian. The terms involving time-odd densities vanish identically in the ground-state of even-even nuclei but increase the computing task for odd-mass nuclei. As discussed for e.g. in Refs. [25, 26], the time-odd densities cause a spin polarisation of the even-even core nucleus which results in the removal of the Kramers degeneracy of the single-particle states. Moreover, the recent work of Ref. [27] shows that the magnetic properties of deformed odd-mass nuclei can be properly described when taking into account the effect of core polarisation due to the breaking of the time-reversal symmetry in the mean-field level. Therefore, it is expected to be more appropriate to take into account the time-reversal symmetry breaking in the study of fission-barrier calculations.

In this work, the mean-field treatment of odd-mass nuclei is based on the Hartree-Fock-plus-BCS (HF+BCS) approach with self-consistent blocking (SCB). The nuclear part of the resulting energy-density functional is parametrized in the two-body density-dependent Skyrme form for the particle-hole channel and the seniority form for the particle-particle channel. The exchange terms induced by the Coulomb interaction are treated in the Slater approximation, and the one-body (dominant) contribution to the center-of-mass correction is taken into account. Axial symmetry is assumed throughout this work. The resulting mean-field solution then serves as the intrinsic state in the Bohr and Mottelson unified model in which the parity π and the projection of the total angular momentum of the blocked single-particle state on the nuclear symmetry axis K is assumed to correspond to the experimental I^{π} quantum numbers. The blocked configuration corresponding to given K^{π} quantum numbers is obtained by setting to 1 the occupation of the K^{π} single-particle state closest to Fermi level and to 0 the occupation of the conjugate state. It should be stressed that the SCB treatment for odd-mass nucleus has, in addition to treating properly the time-reversal symmetry breaking, the advantage that there is no ambiguity in defining the even-even core nucleus while also having a correct average nucleon number. This was not the case in the one-quasi-particle approach for e.g. in the earlier work of Ref. [28].

Research aim and objectives

As mentioned above, one of the quantity of interest from theoretical calculations which can be compared to experiment is the fission cross section. For odd-mass nuclei, one could expect different cross sections corresponding to the different I^{π} quantum numbers of the fissioning compound nuclei. In order to calculate the fission cross sections, one needs as one of the input, the fission-barrier heights. This work focuses only on the latter quantity in odd-mass nuclei, whereby the fission-barrier heights for various I^{π} quantum numbers of the fissioning nucleus are calculated from a self-consistent blocking procedure assuming $I = K$. While the SCB and the time-reversal symmetry breaking formalism have been developed a long time ago, there are by far no published results on the simultaneous application of both aspects to the calculation of fission barriers and energy spectra of odd-mass nuclei, to the best of our knowledge.

The purpose of this work is then to obtain new results with regards to the fission-barrier heights and energy spectra of odd-mass nuclei with the SCB approach in the HF+BCS framework and taking the time-reversal symmetry breaking at the mean-field level into account. The main objectives of this work are as follows:

- to calculate the deformation energy curves of odd-mass nuclei with various blocked K^{π} configurations from which the fission-barrier heights can be deduced
- to describe the energy spectra of odd-mass nuclei at various deformations, namely at the ground-state and fission-isomeric wells as well as the discrete transition states at the top of the barrier (no intrinsic parity breaking at the mean-field level).

In addition to the above, the fission-barrier heights for different blocked K^{π} configurations will also be compared to its neighbouring even-even nuclei. It is expected that the fission-barrier of odd-mass nuclei to be higher and wider than in even-even nuclei as a consequence of having to follow specific K^{π} quantum numbers along the fission path. The extra barrier energy of odd-mass nuclei referred to as the "specialization energy" has been proposed to explain the relatively longer fission half-life of odd-mass nuclei (in, e.g., Ref. [29]).

Roadmap of the thesis

Before presenting mean-field calculations of fission barriers, a discussion of neutron-induced fission cross sections will be presented in Chapter 2 to give an overview of where this work stands in the wider scope of induced-fission studies. Chapter 3 will be devoted to the theoretical framework of the work, in particular the self-consistent blocking procedure within the HF+BCS formalism as well as the description of the Bohr-Mottelson unified model. Some technical and numerical details will be given in Chapter 4. Then, the results will be presented in two separate chapters. Chapter 5 will be devoted to the spectroscopic properties in the ground-state and fission-isomeric wells of some selected odd-mass nuclei, whereas the results on the fission barriers will be presented in Chapter 6. Finally, conclusions and possible extensions of the work will be given in Chapter 7.