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Walid Younes • Daniel Marc Gogny
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A Microscopic Theory of Fission Dynamics Based on the Generator Coordinate Method

Springer

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The idea of writing a book about the microscopic approach to the fission process had been a longstanding wish of Daniel Gogny. Eventually, he began to sketch an outline for such a book in 2015. Most unfortunately, Daniel did not live long enough to see his project completed. This book is based on the many notes Daniel left. The other two authors of the present version have done their best to preserve the spirit and the detail of the deep thinking that Daniel devoted to the complex problem of implementing a description of fission from first principles.

Daniel entered the French Atomic Energy Commission (CEA) in the mid-1960s on the recommendation of Louis de Broglie who had been his teacher at the University of Paris. There he began to work on the subject of the nucleon-nucleon (NN) interaction. With two collaborators, he first implemented at IPN-Orsay a soft-core parameterization of the realistic NN interaction (the Gogny-Pires-de Tourreil force). Then he invented an original effective NN interaction, of finite range and density dependent, which *he called D1 and became subsequently known all over the world as "the Gogny force". He insisted on his effective force to possess a finite range in order to be able to describe the pairing correlations which play a very important role in nuclei without specific phenomenological parameters. The Gogny force is used till now in numerous studies by many research groups worldwide.*

In subsequent years, Daniel and his team in the Bruyères-le-Châtel CEA laboratory employed the D1 force and its improved version called D1S in numerous studies, which allowed them to describe nucleus ground states and spectra all over the nuclear chart in a purely microscopic way. It was in the late 1970s that Daniel initiated the microscopic description of fission at Bruyères-le-Châtel, which is the topic of this book. This work led in the 1980s to a quite realistic description of actinide fission barriers and, more importantly, to the first microscopic interpretation of the scission process. In parallel, Daniel used the nuclear structure approach based on his NN force to interpret the results of electron and alpha scattering experiments performed at the CEA-Saclay. He also extended this approach in order to come up with the definition of a microscopic nucleon-nucleus optical model and the setting up of a microscopic nuclear reaction model.

After 1984, Daniel applied his theoretical skills and profound thinking to a variety of problems in theoretical physics – mathematical proof of the existence of solutions of the Hartree-Fock equations, description of the non-perturbative structure *of the QCD gluon vacuum, NEET effect in plasmas – as well as a wide range of engineering problems.*

In 2002, Daniel moved to the United States and became a part-time consultant at the Lawrence Livermore National Laboratory (LLNL) in Livermore, California, where he worked with nuclear physicists such as M. S. Weiss and A. K. Kerman. Most importantly, he resumed the work about nuclear fission begun at Bruyères-le-Châtel more than 20 years earlier. With W. Younes as a collaborator, he managed to make enormous progress on this difficult topic, most of which is related in detail in this book.

Daniel has always been recognized as a leading physicist and a particularly clear-minded scientific researcher. He was awarded two prestigious prizes of the French scientific community: the Joliot-Curie Prize of the French Physical Society in 1986, and the Lazare Carnot Prize of the French Academy of Science in 1999. His close collaborators as well as his friends and colleagues all over the world will remember his legendary good-naturedness, humour, elegance and evening dinner parties. He is missed by all the persons who had the privilege to work and live close to him, particularly the other two authors of this book.

Preface

The development of a predictive and quantitative theory of fission remains one of the most daunting challenges in nuclear physics. Interest in the theory of fission spans 75 years, starting from the first theoretical approach by Bohr and Wheeler [1], which gave the basic picture of fission as that of a nucleus elongating to its breaking point, to later calculations which include dynamical aspects through the use of time-dependent Hartree-Fock [2], Langevin theory [3–5], Brownian motion [6, 7], and microscopic descriptions based on the time-dependent generator coordinate method [8–11].

A proper microscopic description of fission (i.e., starting from the nucleon degrees of freedom) brings with it all the known complexities of the quantum many-body problem [12], with the additional difficulties of describing the scission of the parent nucleus into two or more fragments within a quantum-mechanical context [13]. This book presents a quantum-mechanical description of the induced nuclear fission process from an initial compound state to scission, starting from protons, neutrons, and an effective interaction between them. This is an ambitious program that raises a host of fundamental questions such as the following: What are the relevant degrees of freedom throughout the process? How do the collective and intrinsic degrees couple during the fission process? How does a nucleus divide into two separate daughters in a quantum-mechanical description where its wave function can be non-local? How is the energy of the fissioning nucleus partitioned between the kinetic and excitation energies of its daughters? These and other questions about fission are currently being investigated through a variety of theoretical, computational, and experimental techniques that are generating a growing body of literature.

For a broad overview of various theoretical approaches to nuclear fission, the reader can consult the recent textbook by Krappe and Pomorski [14]. For a more specialized discussion of microscopic methods, we recommend the very thorough review by Schunck and Robledo [15]. In this manuscript, we will focus in greater detail on the approach originally developed in the 1980s at the Bruyères-le-Châtel laboratory in France, which uses a collective Schrödinger-like equation derived from the time-dependent generator coordinate method, with ingredients built from constrained Hartree-Fock-Bogoliubov solutions. The term "microscopic" in the present context refers to an approach that starts from protons, neutrons, and an effective (i.e., in-medium) interaction between them. The form of this interaction is inspired by more fundamental theories of nuclear matter but still contains parameters that have to be adjusted to data. However, these parameters were adjusted once and for all, and not tuned to reproduce the particular fission observables we will be discussing. The appeal of a microscopic approach is that it does not contain any parameters that depend on the mass, charge, configuration, etc. of the nucleus. This is especially important in the case of fission studies where the parent nucleus eventually splits into two (or more) very different daughter nuclei. In addition, a microscopic approach allows both single-particle and collective degrees of freedom to be treated in a consistent manner. In this way, while the motion of individual nucleons can be described by a mean field, oscillations of this mean field about an equilibrium solution can provide the collective excitations of the system. Finally, the microscopic approach provides a natural description of the approach to scission as a progressive localization of the individual nucleons on the respective nascent fragments and mitigates the otherwise jarring jump that would occur if we had to switch abruptly from a one-body to a two-body formalism. To be sure, the microscopic approach presented in this work is far from complete, but we felt that sufficient progress had been made to warrant taking stock of what has been accomplished so far.

The book is divided into two parts. The first part covers the mathematical tools used in our preferred approach to the fission problem. Chapter 1 gives a detailed overview of the formalism for a microscopic approach to the nuclear many-body problem. The chapter gives a general introduction to the Hartree-Fock-Bogoliubov theory with multiple constraints. The formalism is specialized to the case of a finite-range interaction in Chap. 2. Next, in Chap. 3, the generator coordinate method is presented to construct a collective Hamiltonian from the underlying single-particle degrees of freedom, and the technique is extended to include the coupling between collective and intrinsic motion of the nucleus. Finally, the limiting adiabatic case is considered and the time-dependent treatment of the problem is discussed. The tools and techniques presented in this chapter have much wider applicability than to the fission problem alone, and we have strived to present them in a self-contained pedagogical manner. The second part of the book specializes the discussion to the fission problem. In Chap. 4, the question of the choice of collective coordinates appropriate for the fission process is explored. The description of scission is then studied within a quantum-mechanical context, along with the theory and practical aspects of calculating fission-fragment mass and energy distributions. The particular case of induced fission from ^{240}Pu is presented in detail in Chap. 5 to extract the energies and mass distributions of its primary fragments. Finally in Chap. 6, we take a broader view of the microscopic approach to the fission problem and look at potential future directions in this field. In addition to presenting the research, we have sought to make this book more pedagogical by illustrating some of the concepts in Part I by applying them to a relatively simple toy model of the nucleus, and by expanding the discussion in a series of appendices at the end of the book.

This book is intended as a reference for advanced graduate students and researchers in fission theory. It is also written for practitioners in the field who find themselves frustrated by the paucity of information which is often unavoidable in page-restricted scholarly articles. Therefore, we have included illustrative examples throughout the text to hopefully make it easier for the reader to understand, implement, and verify the formalism that is presented here. Two of the authors, D. Gogny and J. F. Berger, began this work in the 1980s with W. Younes joining the effort in 2006. All three of us have a long-standing interest in the beautiful complexity of the fission process and in trying to understand it as an emergent phenomenon from the underlying nucleon degrees of motion. Sadly D. Gogny passed away in May 2015, when this book was still in its early stages, but his presence and influence is on every page.

Livermore, USA — Walid Younes
Leudeville, France — Jean-François Berger
April 2017

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