

Lecture Notes in Physics

Volume 950

Founding Editors

W. Beiglböck
J. Ehlers
K. Hepp
H. Weidenmüller

Editorial Board

M. Bartelmann, Heidelberg, Germany
P. Hänggi, Augsburg, Germany
M. Hjorth-Jensen, Oslo, Norway
R.A.L. Jones, Sheffield, UK
M. Lewenstein, Barcelona, Spain
H. von Löhneysen, Karlsruhe, Germany
A. Rubio, Hamburg, Germany
M. Salmhofer, Heidelberg, Germany
W. Schleich, Ulm, Germany
S. Theisen, Potsdam, Germany
D. Vollhardt, Augsburg, Germany
J.D. Wells, Ann Arbor, USA
G.P. Zank, Huntsville, USA

The Lecture Notes in Physics

The series Lecture Notes in Physics (LNP), founded in 1969, reports new developments in physics research and teaching—quickly and informally, but with a high quality and the explicit aim to summarize and communicate current knowledge in an accessible way. Books published in this series are conceived as bridging material between advanced graduate textbooks and the forefront of research and to serve three purposes:

- to be a compact and modern up-to-date source of reference on a well-defined topic
- to serve as an accessible introduction to the field to postgraduate students and nonspecialist researchers from related areas
- to be a source of advanced teaching material for specialized seminars, courses and schools

Both monographs and multi-author volumes will be considered for publication. Edited volumes should, however, consist of a very limited number of contributions only. Proceedings will not be considered for LNP.

Volumes published in LNP are disseminated both in print and in electronic formats, the electronic archive being available at springerlink.com. The series content is indexed, abstracted and referenced by many abstracting and information services, bibliographic networks, subscription agencies, library networks, and consortia.

Proposals should be sent to a member of the Editorial Board, or directly to the managing editor at Springer:

Christian Caron
Springer Heidelberg
Physics Editorial Department I
Tiergartenstrasse 17
69121 Heidelberg/Germany
christian.caron@springer.com

More information about this series at <http://www.springer.com/series/5304>

Walid Younes • Daniel Marc Gogny
Jean-François Berger

A Microscopic Theory of Fission Dynamics Based on the Generator Coordinate Method

 Springer

Walid Younes
Department of Physics
Lawrence Livermore National Laboratory
Livermore, CA, USA

Daniel Marc Gogny (deceased)
Lawrence Livermore National Laboratory
Livermore, CA, USA

Jean-François Berger
Centre DAM-Ile de France
Retired from Commissariat à l'Energie
Atomique
Bruyères-le-Châtel, Arpajon, France

This document was prepared as an account of work sponsored by an agency of the US Government. Neither the US Government nor Lawrence Livermore National Security, LLC, nor any of their employees makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the US Government or Lawrence Livermore National Security, LLC. The views and opinions of authors expressed herein do not necessarily state or reflect those of the US Government or Lawrence Livermore National Security, LLC, and shall not be used for advertising or product endorsement purposes.

This work performed under the auspices of the US Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

This book was prepared, either in whole or in part, by a contractor of the U.S. Government under contract number DE-AC52-06NA27344. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

ISSN 0075-8450

ISSN 1616-6361 (electronic)

Lecture Notes in Physics

ISBN 978-3-030-04422-0

ISBN 978-3-030-04424-4 (eBook)

<https://doi.org/10.1007/978-3-030-04424-4>

Library of Congress Control Number: 2018962930

© Springer Nature Switzerland AG 2019

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

The publisher, the authors, and the editors are safe to assume that the advice and information in this book are believed to be true and accurate at the date of publication. Neither the publisher nor the authors or the editors give a warranty, express or implied, with respect to the material contained herein or for any errors or omissions that may have been made. The publisher remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

This Springer imprint is published by the registered company Springer Nature Switzerland AG
The registered company address is: Gewerbestrasse 11, 6330 Cham, Switzerland

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 Turreil 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 DIS 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
Leudeville, France
April 2017

Walid Younes
Jean-François Berger

References

1. Bohr, N., Wheeler, J.A.: Phys. Rev. **56**, 426 (1939)
2. Negele, J.W., Koonin, S.E., Möller, P., Nix, J.R., Sierk, A.J.: Phys. Rev. **17**, 1098 (1978)
3. Borunov, M.V., Nadochty, P.N., Adeev, G.D., Nucl. Phys. **A799**, 56 (2008)
4. Karpov, A.V., Nadochty, P.N., Vanin, D.V., Adeev, G.D.: Phys. Rev. C **63**, 054610 (2001)
5. Nadochty, P.N., Kelic, A., Schmidt, K.-H.: Phys. Rev. C **75**, 064614 (2007)
6. Randrup, J., Möller, P.: Phys. Rev. Lett. **106**, 132503 (2011)
7. Randrup, J., Möller, P., Sierk, A.J.: Phys. Rev. C **84**, 034613 (2011)
8. Berger, J.-F., Girod, M., Gogny, D.: Nucl. Phys. **A428**, 23c (1984)
9. Berger, J.F., Girod, M., Gogny, D.: Nucl. Phys. **A502**, 85 (1989)
10. Berger, J.F., Girod, M., Gogny, D.: Comput. Phys. Commun. **63**, 365 (1991)
11. Goutte, H., Berger, J.-F., Casoli, P., Gogny, D.: Phys. Rev. C **71**, 024316 (2005)
12. Aaronson, S.: Nat. Phys. **5**, 707 (2009)
13. Younes, W., Gogny, D.: Phys. Rev. Lett. **107**, 132501 (2011)
14. Krappe, H.J., Pomorski, K.: Theory of Nuclear Fission. Springer, Heidelberg (2012)
15. Schunck, N., Robledo, L.M.: Submitted to Rep. Prog. Phys. (2016). arXiv:1511.07517v2

Contents

Part I Tools for a Microscopic Theory of the Nucleus

1	Hartree-Fock-Bogoliubov Theory	3
1.1	General Formalism	3
1.2	Perturbation of the Generalized Density Matrix Around the HFB Solution	10
1.3	Stability of the HFB Vacuum and Definition of the QRPA Matrix	12
1.4	Response of HFB to a One-Body External Field	23
1.5	HFB with Additional Constraints	27
1.5.1	The Case of One Constraint	28
1.5.2	The Case of N Constraints	29
1.6	Illustration of the Constrained HFB Method with the Multi- O (4) Model	30
1.6.1	Description of the Model	31
1.6.2	Constrained Hartree-Fock-Bogoliubov Calculations	32
	References	39
2	Matrix Elements of the Finite-Range Interaction	41
2.1	General Form of the Interaction	41
2.2	The Deformed Harmonic-Oscillator Basis	42
2.3	Form of the HFB Equations	45
2.3.1	Total Energy of the System	45
2.3.2	The Hartree-Fock Field	48
2.3.3	The Pairing Field	49
2.4	Matrix Elements in an Axially Deformed Harmonic-Oscillator Basis	50
2.4.1	Matrix Element of the Kinetic-Energy Operator	50
2.4.2	Matrix Elements of the Central Contribution	51
2.4.3	Matrix Elements of the Coulomb Contribution	55
2.4.4	Matrix Elements of the Spin-Orbit Contribution	61
2.4.5	Two-Body Center-of-Mass Correction	70

2.4.6	The Density-Dependent Contribution	75
2.4.7	The Slater Approximation to the Coulomb Exchange Term	77
	References	78
3	The Generator Coordinate Method	79
3.1	The Hill-Wheeler Equation	80
3.1.1	General Formalism	80
3.1.2	Calculation of GCM Kernels	85
3.1.3	Discrete-Basis Hill-Wheeler Method Without Projection ...	89
3.1.4	Particle-Number Projected Discrete Hill-Wheeler Calculations	92
3.2	A Collective Schrödinger Equation in the Adiabatic Limit	97
3.2.1	Reduction of the Hill-Wheeler Equation to a Bohr-Like Hamiltonian	97
3.2.2	Calculation of the Inertia Tensor	110
3.3	The Schrödinger Collective Intrinsic Model	137
3.3.1	General Formalism	137
3.3.2	Calculation of $\hat{J}_{-1/2}(\bar{q})$ in the One-Dimensional Case	140
3.3.3	A Schrödinger-Like Equation	150
3.3.4	Illustration with the Multi- $O(4)$ Model	157
	References	172
 Part II Application to Low-Energy Fission		
4	General Concepts	177
4.1	The Choice of Collective Constraints	177
4.1.1	Multipole-Moment Constraints	177
4.1.2	Constraints on the Pre-fragments	178
4.2	A Quantum Mechanical Picture of Scission	183
4.2.1	Quantum Localization	184
4.2.2	Energy Partition	186
4.2.3	Scission Criteria	188
4.2.4	Description of the Nucleus Beyond Scission	190
4.3	Calculation of Fragment Mass Distributions	191
4.3.1	The Collective Hamiltonian	191
4.3.2	The Direction of Fission in the Dynamical Calculations ...	192
4.3.3	From Flux to Fragment Mass Distribution	195
4.4	Calculation of Fragment Energies	198
4.4.1	Static Contribution	198
4.4.2	Dynamical Contribution	199
	References	202
5	Numerical Application to ^{240}Pu Fission	205
5.1	Potential Energy Surface and Inertia Tensor	205
5.2	Initial States	206

5.3	Fragment Mass Distribution	209
5.4	Fragment Energies.....	209
	References	212
6	Summary and Outlook for Future Directions in Fission Theory	213
6.1	Concluding Remarks About the Methods Presented in This Work	213
6.2	Survey of Other Fission-Theory Approaches	215
6.2.1	Statics	215
6.2.2	Dynamics	220
6.2.3	Data Evaluations.....	230
	References	232
	Appendix A Hartree-Fock-Bogoliubov Algorithm	237
	References	238
	Appendix B Exact Solution of the Multi-O (4) Model	239
B.1	Useful Results for the Quasi-spin Algebra	241
B.1.1	The Action of \hat{K}_j^0 on the State $(\hat{K}_j^+)^n 0\rangle$	241
B.1.2	The Action of \hat{K}_j^- on the State $(\hat{K}_j^+)^n 0\rangle$	242
B.1.3	Normalization of the State $(\hat{K}_j^+)^n 0\rangle$	243
B.2	Many-Body Basis States	244
B.3	Matrix Elements of the Model Hamiltonian	245
B.4	Transition Matrix Elements	248
B.5	Numerical Example and Discussion.....	248
	References	250
	Appendix C Projection on Particle Number	251
C.1	Different Formulations of the Bogoliubov Vacuum	251
C.2	A “Pedestrian” Approach	252
C.2.1	Illustration with a Simple Example	253
C.2.2	Normalization.....	254
C.2.3	One-Body Density Matrix.....	255
C.2.4	Two-Body Density Matrix	257
C.2.5	Projected Expectation Value of the Two-Body Potential ...	260
C.3	A Projection Operator on Particle Number.....	262
C.3.1	Basic Definitions	262
C.3.2	Application.....	264
C.4	Another Point of View	265
C.4.1	Alternate Form of the One-Body Density	265
	References	271

Appendix D Particle-Number Projected GCM Matrix Elements	273
D.1 General Results	273
D.2 Norm Overlap	274
D.3 Generalized One-Body Density	281
D.3.1 Preliminary Definitions and Results	281
D.3.2 Projected Matrix Elements of $a^\dagger a$	282
D.3.3 Calculation of the Matrix Elements $\left\langle \Phi_q^{(p)}(\varphi) \left a_\alpha^{q'} a_\beta^{q'} \right \Phi_{q'}^{(p)}(\varphi') \right\rangle$	288
D.3.4 Calculation of the Matrix Elements $\left\langle \Phi_q^{(p)} \left P_q^{(N)\dagger} a_\alpha^{q'\dagger} a_\beta^{q'\dagger} P_{q'}^{(N)} \right \Phi_{q'}^{(p)} \right\rangle$	290
D.4 Application to Hamiltonians	292
Reference	295
Appendix E Symmetric Ordered Products of Operators	297
E.1 Pedestrian Derivation of the SME	297
E.1.1 Basic Formula	297
E.1.2 Derivatives of SOPOs	299
E.1.3 Useful Identities for SOPOs	301
E.1.4 Composition of Two SOPOs	308
E.1.5 Composition of Three SOPO's	310
Reference	314
Appendix F Algorithm for the TDGCM in the Gaussian Overlap Approximation	315
References	316
Appendix G Mathematica Script for Calculating the Coefficients of the Schrodinger-Like Equation	317
Reference	319
Index	321