MATHEMATICAL AND COMPUTATIONAL MODELING

MATHEMATICAL AND COMPUTATIONAL MODELING

With Applications in Natural and Social Sciences, Engineering, and the Arts

Edited by

RODERICK MELNIK
Wilfrid Laurier University
Waterloo, Ontario, Canada

WILEY

Published by John Wiley & Sons, Inc., Hoboken, New Jersey
Published simultaneously in Canada

Library of Congress Cataloging-in-Publication Data:

Mathematical and computational modeling : with applications in natural and social sciences, engineering, and the arts / edited by Roderick Melnik, Wilfrid Laurier University, Waterloo, Ontario, Canada.
pages cm
Includes bibliographical references and index.
ISBN 978-1-118-85398-6 (cloth)
1. Mathematical models. I. Melnik, Roderick, editor.
QA401.M3926 2015
511′.8—dc23
2014043267

Set in 10/12pts Times Lt Std by SPi Publisher Services, Pondicherry, India

Printed in the United States of America

10 9 8 7 6 5 4 3 2 1

1 2015

CONTENTS

PREFACE

Mathematical and computational modeling has become a major driving force in scientific discovery and innovation, covering an increasing range of diverse application areas in the natural and social sciences, engineering, and the arts. Mathematical models, methods, and algorithms have been ubiquitous in human activities from the ancient times till now. The fundamental role they play in human knowledge, as well as in our well-being, is indisputable, and it continues to grow in its importance.

Significant sources of some of the most urgent and challenging problems the humanity faces today are coming not only from traditional areas of mathematics applications in natural and engineering sciences, but also from life, behavioral, and social sciences. We are witnessing an unprecedented growth of model-based approaches in practically every domain of human activities. This expands further interdisciplinary horizons of mathematical and computational modeling, providing new and strengthening existing links between different disciplines and human activities. Integrative, holistic approaches and systems–science methodologies are required in an increasing number of areas of human endeavor. In its turn, such approaches and methodologies require the development of new state-of-the-art mathematical models and methods.

Given this wide spectrum of applications of mathematical and computational modeling, we have selected five representative areas, grouped in this book into sections. These sections contain 12 selective chapters, written by 25 experts in their respective fields. They open to the reader a broad range of methods and tools important in many applications across different disciplines. The book provides details on state-of-the-art achievements in the development of these methods and tools, as well as their applications. Original results are presented on both fundamental theoretical and applied developments, with many examples emphasizing interdisciplinary nature of mathematical and computational modeling and universality of models in our better understanding nature, society, and the man-made world.

Aimed at researchers in academia, practitioners, and graduate students, the book promotes interdisciplinary collaborations required to meet the challenges at the interface of different disciplines on the one hand and mathematical and computational modeling on the other. It can serve as a reference on theory and applications of mathematical and computational modeling in diverse areas within the natural and social sciences, engineering, and the arts.

I am thankful to many of my colleagues in North America, Europe, Asia, and Australia whose encouragements were vital for the completion of this project. Special thanks go to the referees of this volume. Their help and suggestions were invaluable. Finally, I am very grateful to the John Wiley & Sons editorial team, and in particular, Susanne Steitz-Filler and Sari Friedman for their highly professional support.

Waterloo, ON, Canada RODERICK MELNIK
August 2014–2015

1

UNIVERSALITY OF MATHEMATICAL MODELS IN UNDERSTANDING NATURE, SOCIETY, AND MAN-MADE WORLD

Roderick Melnik
The MS2Discovery Interdisciplinary Research Institute, M^{2}NeT Laboratory and Department of Mathematics, Wilfrid Laurier University, Waterloo, Ontario, Canada

1.1 HUMAN KNOWLEDGE, MODELS, AND ALGORITHMS

There are various statistical and mathematical models of the accumulation of human knowledge. Taking one of them as a starting point, the Anderla model, we would learn that the amount of human knowledge about 40 years ago was 128 times greater than in the year A.D. 1. We also know that this has increased drastically over the last four decades. However, most such models are economics-based and account for technological developments only, while there is much more in human knowledge to account for. Human knowledge has always been linked to models. Such models cover a variety of fields of human endeavor, from the arts to agriculture, from the description of natural phenomena to the development of new technologies and to the attempts of better understanding societal issues. From the dawn of human civilization, the development of these models, in one way or another, has always been connected with the development of mathematics. These two processes, the development of models representing the core of human knowledge and the development of mathematics, have always gone hand in hand with each other. From our knowledge

Mathematical and Computational Modeling: With Applications in Natural and Social Sciences, Engineering, and the Arts, First Edition. Roderick Melnik.

in particle physics and spin glasses [4, 6] to life sciences and neuron stars [1, 5, 16], universality of mathematical models has to be seen from this perspective.

Of course, the history of mathematics goes back much deeper in the dawn of civilizations than A.D. 1 as mentioned earlier. We know, for example, that as early as in the 6th–5th millennium B.C., people of the Ancient World, including predynastic Sumerians and Egyptians, reflected their geometric-design-based models on their artifacts. People at that time started obtaining insights into the phenomena observed in nature by using quantitative representations, schemes, and figures. Geometry played a fundamental role in the Ancient World. With civilization settlements and the development of agriculture, the role of mathematics in general, and quantitative approaches in particular, has substantially increased. From the early times of measurements of plots of lands and of the creation of the lunar calendar, the Sumerians and Babylonians, among others, were greatly contributing to the development of mathematics. We know that from those times onward, mathematics has never been developed in isolation from other disciplines. The cross-fertilization between mathematical sciences and other disciplines is what produces one of the most valuable parts of human knowledge. Indeed, mathematics has a universal language that allows other disciplines to significantly advance their own fields of knowledge, hence contributing to human knowledge as a whole. Among other disciplines, the architecture and the arts have been playing an important role in this process from as far in our history as we can see. Recall that the summation series was the origin of harmonic design. This technique was known in the Ancient Egypt at least since the construction of the Chephren Pyramid of Giza in 2500 BCE (the earliest known is the Pyramid of Djoser, likely constructed between 2630 BCE and 2611 BCE). The golden ratio and Fibonacci sequence have deep roots in the arts, including music, as well as in the natural sciences. Speaking of mathematics, H. Poincare once mentioned that "it is the unexpected bringing together of diverse parts of our science which brings progress" [11]. However, this is largely true with respect to other sciences as well and, more generally, to all branches of human endeavor. Back to Poincare's time, it was believed that mathematics "confines itself at the same time to philosophy and to physics, and it is for these two neighbors that we work" [11]. Today, the quantitative analysis as an essential tool in the mathematics arsenal, along with associated mathematical, statistical, and computational models, advances knowledge in pretty much every domain of human endeavor. The quantitative-analysis-based models are now rooted firmly in the application areas that were only recently (by historical account) considered as non-traditional for conventional mathematics. This includes, but not limited to, life sciences and medicine, user-centered design and soft engineering, new branches of arts, business and economics, social, behavioral, and political sciences.

Recognition of universality of mathematical models in understanding nature, society, and man-made world is of ancient origin too. Already Pythagoras taught that in its deepest sense the reality is mathematical in nature. The origin of quantification of science goes back at least to the time of Pythagoras' teaching that numbers provide a key to the ultimate reality. The Pythagorean tradition is well reflected in the Galileo statement that "the *Book of Nature* is written in the language of mathematics." Today, we are witnessing the areas of mathematics applications not only growing rapidly in more traditional natural and engineering sciences but also in social and behavioral sciences as well. It should be noted that the term "universality" is also used in the literature in different, more specific and narrow contexts. For example, in statistical mechanics, universality is the observation that there are properties for a large class of systems that are independent of the dynamical details of the system. A pure mathematical definition of a universal property is usually given based on representations of category theory. Another example is provided by computer science and computability theory where the word "universal" is usually applied to a system which is Turing complete. There is also a universality principle, a system property often modeled by random matrices. These concepts are useful for corresponding mathematical or statistical models and are subject of many articles (see, e.g., [2–7, 14, 16] and references therein). For example, the authors of Ref. [2] discuss universality classes for complex networks with possible applications in social and biological dynamic systems. A universal scaling limit for a class of Ising-type mathematical models is discussed in Ref. [6]. The concept of universality of predictions is discussed in Ref. [14] within the Bayesian framework. Computing universality is a subject of discussions in Ref. [3], while universality in physical and life sciences are discussed in Refs. [7] and [5], respectively. Given a brief historical account demonstrating the intrinsic presence of models in human knowledge from the dawn of civilizations, "universality" here is understood in a more general, Aristotle's sense: "To say of what is, that it is not, or of what is not, that it is, is false; while to say of what is, that it is, and of what is not, that it is not, is true." The underlying reason for this universality lies with the fact that models are inherently linked to algorithms. From the ancient times till now, human activities and practical applications have stimulated the development of model-based algorithms. If we note that abstract areas of mathematics are also based on models, it can be concluded that mathematical algorithms have been at the heart of the development of mathematics itself. The word "algorithm" was derived from Al-Khwarizmi (c. 780 – c. 850), a mathematician, astronomer and geographer, whose name was given to him by the place of his birth (Khwarezm or Chorasmia). The word indicated a technique with numerals. Such techniques were present in human activities well before the ninth century, while specific algorithms, mainly stimulated by geometric considerations at that time, were also known. Examples include algorithms for approximating the area of a given circle (known to Babylonians and Indians), an algorithm for calculating π by inscribing and then circumscribing a polygon around a circle (known to Antiphon and Bryson already in the fifth century B.C.), Euclid's algorithm to determine the greatest common divisor of two integers, and many others. Further development of the subject was closely interwoven with applications and other disciplines. It led to what in the second part of the twentieth century was called by E. Wigner as "the unreasonable effectiveness of mathematics in the natural sciences." In addition to traditional areas of natural sciences and engineering, the twentieth century saw an ever increasing role of mathematical models in the life and environmental sciences too. This development was based on earlier achievements. Indeed, already during the 300 B.C., Aristotle studied the manner in which species evolve to fit their environment. His works served as an important stepping stone in the development of modern evolutionary theories, and his holistic views and teaching that revolutionized many branches of mathematics. Game theory and the developments in control and cybernetics were influenced by the developments in social, behavioral, and life sciences, while the growth of systems science has provided one of the fundamentals for the development of systems biology where biological systems are considered in a holistic way [1]. There is a growing understanding that the interactions between different components of a biological system at different scales (e.g., from the molecular to the systemic level) are critical. Biological systems provide an excellent example of coupled systems and multiscale dynamics. A multiscale spatiotemporal character of most systems in nature, science, and engineering is intrinsic, demonstrating complex interplay of its components, well elucidated in the literature (e.g., [8, 9, 13] and references therein). In life sciences, the number of such examples of multiscale coupled systems and associated problems is growing rapidly in many different, albeit often interconnected, areas. Some examples are as follows:

- Complex biological networks, genomics, cellular systems biology, and systems biological approaches in other areas, studies of various organs, their systems, and functions;
- Brain dynamics, neuroscience and physiology, developmental biology, evolution and evolutionary dynamics of biological games;
- Immunology problems, epidemiology and infectious diseases, drug development, delivery, and resistance;
- Properties, dynamics, and interactions at various length and time scales in bio-macromolecules, including DNA, RNA, proteins, self-assembly and spatiotemporal pattern formation in biological systems, phase transitions, and so on.

Many mathematical and computational modeling tools are ubiquitous. They are universal in a sense that they can be applied in many other areas of human endeavors. Life sciences have a special place when we look into the future developments of mathematical and computational modeling. Indeed, compared to other areas, for example, those where we study physical or engineering systems, our knowledge of biological systems is quite limited. One of the reasons behind this is biological system complexity, characterized by the fact that most biological systems require dealing with multiscale interactions of their highly heterogeneous parts on different time scales.

In these cases in particular, the process of mathematical and computational modeling becomes frequently a driving source for the development of hierarchies of mathematical models. This helps determine the range of applicability of models. What is especially important is that based on such hierarchies, mathematical models can assist in explaining the behavior of a system under different conditions and the interaction of different system components. Clearly, different models for the same system can involve a range of mathematical structures and can be formalized with various mathematical tools such as equation- or inequality-based models, graphs, and logical and game theoretic models. We know by now that the class of the models amenable to analytical treatments, while keeping assumptions realistic, is strikingly small, when compared to the general class of mathematical models that are at the forefront of modern science and engineering [10]. As a result, most modern problems are treated numerically, in which case the development of efficient algorithms becomes critical. As soon as such algorithms are implemented on a computer, we can run the model multiple times under varying conditions, helping us to answer outstanding questions quicker and more efficiently, providing us an option to improve the model when necessary. Model-algorithm-implementation is a triad which is at the heart of mathematical modeling and computational experiment. It is a pervasive, powerful, theoretical, and practical tool, covering the entire landscape of mathematical applications [10]. This tool will play an increasingly fundamental role in the future as we can carry out mathematical modeling and computational experiment even in those cases when natural experiments are impossible. At the same time, given appropriate validation and verification procedures, we can provide reliable information more quickly and with less expense compared to natural experiments. The two-way interactions between new developments in information technology and mathematical modeling and computational experiment are continuously increasing predictive capabilities and research power of mathematical models.

Looking into the future from a modeling perspective, we should also point out that such predictive capabilities and research power allow us to deal with complex systems that have intrinsically interconnected (coupled) parts, interacting in nontrivial dynamic manner. In addition to life, behavioral, and social sciences, mentioned earlier, such systems arise in many other areas, including, but not limited to, fusion and energy problems, materials science and chemistry, high energy and nuclear physics, cosmology and astrophysics, earth, climate, environmental, and sustainability sciences.

In addition to the development of new models and efficient algorithms, the success of predictive mathematical modeling in applications is dependent also on further advances in information sciences and the development of statistical, probabilistic, and uncertainty quantification methods. Uncertainty comes from many different sources, among which we will mention parameters with uncertain values, uncertainty in the model as a representation of the underlying phenomenon, process, or system, and uncertainty in collecting/processing/measurements of data for model calibration. The task of quantifying and mitigating these uncertainties in mathematical models leads to the development of new statistical/stochastic methods, along with methods for efficient integration of data and simulation.

Further to supporting theories and increasing our predictive capabilities, mathematical and computational modeling can often suggest sharper natural experiments and more focused observations, providing in their turn a check to the model accuracy. Natural experiments and results of observations may produce large amounts of data sets that can intelligently be processed only with efficient mathematical data mining algorithms, and powerful statistical and visualization tools [15]. The application of these algorithms and tools requires a close collaboration between different disciplines. As a result, observations and experiments, theory and modeling reinforce each other, leading together to our better understanding of phenomena, processes, and systems we study, as well as to the necessity of even more close interactions between mathematical modeling, computational analyses, and experimental approaches.

1.3 WHAT THIS BOOK IS ABOUT

The rest of the book consists of 4 main sections, containing 11 state-of-the-art chapters on applications of mathematical and computational modeling in natural and social sciences, engineering, and the arts. These chapters are based on selected invited contributions from leading specialists from all over the world. Inevitably, given the vast range of research areas within the field of mathematical and computational modeling, the book such as this can present only selective topics. At the same time, these selective topics open to the reader a broad spectrum of methods and tools important in these applications, and ranging from infectious disease dynamics and epidemic modeling to superconductivity and quantum mechanical challenges, from the models for voting systems to the modeling of musical rhythms. The book provides both theoretical advances in these areas of applications, as well as some representative examples of modern problems from these applications. Following this introductory section, each remaining section with its chapters stands alone as an in-depth research or a survey within a specific area of application of mathematical and computational modeling. We highlight the main features of each such chapter within four main remaining sections of this book.

- **Advanced Mathematical and Computational Models in Physics and Chemistry.** This section consists of three chapters.

  – This section is opened by a chapter written by I. M. Sigal who addresses the macroscopic theory of superconductivity. Superconducting vortex states provide a rich area of research. In the 1950s A. Abrikosov solved the Ginzburg–Landau (GL) equations in an applied magnetic field for certain values of GL parameter (later A. Abrikosov received a Nobel Prize for this work). This led to what is now known as the famous vortex solution, characterized by the fact that the superconducting order parameter contains a periodic lattice of zeros. In its turn, this led to studies of a new mixed Abrikosov vortex phase between the Meissner state and the normal state. The area keeps generating new interesting results in both theory and application. For example, unconventional vortex pattern formations (e.g., vortex clustering) were recently discovered in multiband superconductors (e.g., [17] and references therein). Such phenomena, which are of both fundamental and practical significance, present a subject of many experimental and theoretical works. Recently, it was shown that at low temperatures the vortices form an ordered Abrikosov lattice both in low and in high fields. The vortices demonstrate distinctive modulated structures at intermediate fields depending on the effective intervortex attraction. These and other discoveries generate an increasing interest to magnetic vortices and Abrikosov lattices. Chapter by I. M. Sigal reminds us that the celebrated GL equations form an integral part, namely the Abelian-Higgs component, of the standard model of particle physics, having fundamental consequences for many areas of physics, including those beyond the original designation area of the model. Not only this chapter reviews earlier works on key solutions of the GL model, but it presents some interesting recent results. Vortex lattices, their existence, stability, and dynamics are discussed, demonstrating also that automorphic functions appear naturally in this context and play an important role.

– A prominent role in physics and chemistry is played by the Hartree-Fock method which is based on an approximation allowing to determine the wave function and the energy of a quantum many-body system in a stationary state. More precisely, the Hartree-Fock theoretical framework is based on the variational molecular orbital theory, allowing to solve Schrödinger's equation in such a way that each electron spatial distribution is described by a single, one-electron wave function, known as molecular orbital. While in the classical Hartree-Fock theory the motion of electrons is uncorrelated, correlated wavefunction methods remedy this drawback. The second chapter in this section is devoted to a multireference local correlation framework in quantum chemistry, focusing on numerical challenges in the Cholesky decomposition context. The starting point of the discussion, presented by D. K. Krisiloff, J. M. Dieterich, F. Libisch, and E. A. Carter, is based on the fact that local correlation methods developed for solving Schrödinger's equation for molecules have a reduced computational cost compared to their canonical counterparts. Hence, the authors point out that these methods can be used to model notably larger chemical systems compared to the canonical algorithms. The authors analyze in detail local algorithmic blocks of these methods.

– Variational methods are in the center of the last chapter of this section, written by M. Levy and A. Gonis. The basic premises here lie with the Rayleigh-Ritz variational principle which, in the context of quantum mechanical applications, reduces the problem of determining the ground-state energy of a Hamiltonian system consisting of N interacting electrons to the minimization of the energy functional. The authors then move to the main part of their results, closely connected to a fundamental element of quantum mechanics. In particular, they provide two alternative proofs of the generalization of the variational theorem for Hamiltonians of N-electron systems to wavefunctions of dimensions higher than N. They also discuss possible applications of their main result.

• **Mathematical and Statistical Models in Life Science Applications.** This section consists of two chapters.

– The first chapter deals with mathematical modeling of infectious disease dynamics, control, and treatment, focusing on a model for the spread of tuberculosis (TB). TB is considered to be the second highest cause of infectious disease-induced mortality after HIV/AIDS. Written by J. Arino and I. A. Soliman, this chapter provides a detailed account of a model that incorporates three strains, namely (1) drug sensitive, (2) emerging multidrug resistant, and (3) extensively drug-resistant. The authors provide an excellent introduction to the subject area, followed by the model analysis. In studying the dynamics of the model, they characterize parameter regions where backward bifurcation may occur. They demonstrate the global stability of the disease-free equilibrium in regions with no backward bifurcation. In conclusion, the authors discuss possible options for their model improvement and how mathematical epidemiology contributes to our better understanding of disease transmission processes and their control.

– Epidemiological modeling requires the development and application of an integrated approach. The second chapter of this section focuses on these issues with emphasis on antibiotic resistance. The chapter is written by E. Y. Klein, J. Chelen, M. D. Makowsky, and P. E. Smaldino. They stress the importance of integrating human behavior, social networks, and space into infectious disease modeling. The field of antibiotic resistance is a prime example where this is particularly critical. The authors point out that the annual economic cost to the US health care system of antibiotic-resistant infections is estimated to be $21–$34 billion, and given human health and economics reasons, they set a task of better understanding how resistant bacterial pathogens evolve and persist in human populations. They provide a selection of historical achievements and limitations in mathematical modeling of infectious diseases. This is followed by a discussion of the integrated approach, the authors advocate for, in addressing the multifaceted problem of designing innovative public health strategies against bacterial pathogens. The interaction of epidemiological, evolutionary, and behavioral factors, along with cross-disciplinary collaboration in developing new models and strategies, is becoming crucial for our success in this important field.

• **Mathematical Models and Analysis for Science and Engineering.** This section consists of four chapters.

– The first chapter is devoted to mathematical models in climate modeling, with a major focus given to examples from climate atmosphere-ocean science (CAOS). However, it covers potentially a much larger area of applications in science and engineering. Indeed, as pointed out by the authors of this chapter, D. Giannakis and A. J. Majda, large-scale data sets generated by dynamical systems arise in a vast range of disciplines in science and engineering, for example, fluid dynamics, materials science, astrophysics, earth sciences, to name just a few. Therefore, the main emphasis of this chapter is on data-driven methods for dynamical systems, aiming at quantifying predictability and extracting spatiotemporal patterns. In the context of CAOS, we are dealing with a system of time-dependent coupled nonlinear PDEs. The dynamics of this system takes place in an infinite-dimensional phase space, where the corresponding equations of fluid flow and thermodynamics are defined. In this case, the observed data usually correspond to well-defined physical functions of that phase space, for example, temperature, pressure, or circulation, measured over a set of spatial points. Data-driven methods appear to be critical in considered a case where there are no political parties, as well as a number of other possible cases. Their system elects the set of candidates that maximizes the satisfaction of all voters, where a candidate's satisfaction score is the sum of the satisfactions that her/his election would give to all voters, while a voter's satisfaction is the fraction of her/his approved candidates who are elected. The authors demonstrated that SAV and AV may elect disjoint sets of candidates. In this context, an example of a recent election of the Game Theory Society was given. In conclusion, the authors explained why the most compelling application of their SAV is to party-list systems. This observation has important social implications because SAV is likely to lead to more informed voting and more responsive government in parliamentary systems.

– The concluding chapter of this section and the book provides an example of application of mathematical methods to arts, focusing on music, an art form whose medium is sound and silence. Ancient civilizations, including Egyptians, Chinese, Indian, Mesopotamians, and Greek, studied mathematics of sound. The expression of musical scales in terms of the ratios of small integers goes deep into the human history. Harmony arising out of numbers was sought in all natural phenomena by the Ancient Greeks, starting from Pythagoras. The word "harmonikos" was reserved in that time for those skilled in music. Nowadays, we use the word "harmonics" indicating waves with frequencies that are integer multiples of one another. The applications of mathematical methods from number theory, algebra, and geometry in music are well known, as well as the incorporation of Fibonacci numbers and the golden ratio in musical compositions. The concluding chapter, written by G. T. Toussaint, is devoted to the field of evolutionary musicology where one concerns with characterizing what music is, determining its origin and cross-cultural universals. The author notes that a phylogeny of music may sometimes be correctly constructed from rhythmic features alone. Then, a phylogenetic analysis of a family of rhythms can be carried out based on dissimilarity matrix that is calculated from all pairs of rhythms in the family. How do we define musical rhythms? How do we analyze them? Asking these questions, the author provides a comprehensive account to what is known in this field, focusing on the mathematical analysis of musical rhythms. The working horse of the discussion is the well-known *clave son* rhythm popular in many cultures around the world. The main methodology developed for the analysis is based on geometric quantization. Different types of models are considered and compared, highlighting most important musicological properties.

1.4 CONCLUDING REMARKS

Mathematical and computational modeling, their methods, and tools are rapidly becoming a major driving force in scientific discovery and innovation, providing us with increasingly more reliable predictive capabilities in many areas of human endeavor. In this section, we have presented a brief historical account and an overview of new trends in this field, demonstrating universality of mathematical models. We highlighted a unique selection of topics, representing part of a vast spectrum of the interface between mathematics and its applications, that are discussed in detail in subsequent sections of the book. These topics cover mathematical and computational models from natural and social sciences, engineering, and the arts.

REFERENCES

1. Antoniouk, A. and Melnik, R. (Eds), Mathematics and life sciences, Berlin, De Gruyter, 2012.
2. Barzel, B. and Barabasi, A. L., Universality in network dynamics, Nature Physics, 9 (10), 673–681 (2013).
3. Burgin, M. and Eberbach, E., Universality for turing machines, inductive turing machines and evolutionary algorithms, Fundamenta Informaticae, 91 (1), 53–77 (2009).
4. Carmona, P. and Hu, Y. Y., Universality in Sherrington-Kirkpatrick's spin glass model, Annales de L'Institut Henri Poincare - Probabilities et Statistiques, 42 (2), 215–222 (2006).
5. Chay, T. R., Fan, Y. S., and Lee, Y. S., Bursting, spiking, chaos, fractals, and universality in biological rhythms, International Journal of Bifurcation and Chaos, 5 (3) 595–635 (1995).
6. Chelkak, D. and Smirnov, S., Universality in the 2D Ising model and conformal invariance of fermionic observables, Inventiones Mathematicae, 189 (3), 515–580 (2012).
7. Dolan, B. P., Modular invariance, universality and crossover in the quantum Hall effect, Nuclear Physics B, 554 (3), 487–513 (1999).
8. Engquist, B., Lötstedt, P., and Runborg, O. (Eds.), Multiscale modeling and simulation in science, Berlin; Springer, 2009.
9. Foster, D. H., Costa, T., Peszynska, M., and Schneider, G., Multiscale modeling of solar cells with interface phenomena, Journal of Coupled Systems and Multiscale Dynamics, 1, 179–204 (2013).
10. Melnik, R. and Kotsireas, I. (Eds), Advances in applied mathematics, modeling, and computational science, Fields Institute Communications, 66, New York, Springer, 2013.
11. Poincare, H., L'avenir des mathématiques ("The Future of Mathematics"). Revue générale des sciences pures et appliquées, 19 (23), 930–939 (1908).
12. Rapoport, A., Mathematical models in the social and behavioral sciences, New York, John Wiley & Sons, Inc., 1983.
13. Regenauer-Lieb, K., Veveakis, M., Poulet, T., et al., Multiscale coupling and multi-physics approaches in earth sciences: Theory, Journal of Coupled Systems and Multiscale Dynamics, 1, 49–73 (2013).
14. Sancetta, A., Universality of Bayesian predictions, Bayesian Analysis, 7 (1), 1–36 (2012).
15. Sokolowski, J. A. and Banks, C. M., Modeling and simulation fundamentals: theoretical underpinnings and practical domains, Hoboken, NJ, John Wiley & Sons, Inc., 2010.
16. Tsui, L. K. and Leung, P. T., Universality in quasi-normal modes of neutron stars, Monthly Notices of the Royal Astronomical Society, 357 (3), 1029–1037 (2005).
17. Xu, X. B., Fangohr, H., Gu, M., et al., Simulation of the phase diagram of magnetic vortices in two-dimensional superconductors: evidence for vortex chain formation, Journal of Physics - Condensed Matter, 26 (11), 115702 (2014).

SECTION 1

INTRODUCTION

2

MAGNETIC VORTICES, ABRIKOSOV LATTICES, AND AUTOMORPHIC FUNCTIONS

Israel Michael Sigal
Department of Mathematics, University of Toronto, Ontario, Canada

2.1 INTRODUCTION

In this chapter, we present some recent results on the Ginzburg–Landau equations of superconductivity and review appropriate background. The Ginzburg–Landau equations describe the key mesoscopic and macroscopic properties of superconductors and form the basis of the phenomenological theory of superconductivity. They are thought of to be the result of coarse-graining the Bardeen–Cooper–Schrieffer microscopic model, and were derived from that model by Gorkov [36]. (Recently, the rigorous derivation in the case of nondynamic magnetic fields was achieved by Frank et al. [34].)

These equations appear also in particle physics, as the Abelean-Higgs model, which is the simplest, and arguably most important, ingredient of the standard model [93]. Geometrically, they are the simplest equations describing the interaction of the electromagnetic field and a complex field, and can be thought of as the 'Dirichlet' problem for a connection of $U(1)-$principal bundle and a section of associated vector bundle.

One of the most interesting mathematical and physical phenomena connected with Ginzburg–Landau equations is the presence of *vortices* in their solutions. Roughly speaking, a vortex is a spatially localized structure in the solution, characterized by

Mathematical and Computational Modeling: With Applications in Natural and Social Sciences, Engineering, and the Arts, First Edition. Roderick Melnik.

One of the analytically interesting aspects of the Ginzburg–Landau theory is the fact that, because of the gauge transformations, the symmetry group is infinite-dimensional.

2.2.3 Quantization of flux

Consider first finite energy states (Ψ, A) that have the regularity $H^2_{\text{loc}}(\mathbb{R}^2)$ of solutions to (2.1) (see Ref. [15] for the regularity results). Such states are classified by their topological degree (the winding number of ψ at infinity):

$$\deg(\Psi) := \text{degree}\left(\left.\frac{\Psi}{|\Psi|}\right|_{|x|=R} : \mathbb{S}^1 \to \mathbb{S}^1 \right),$$

for $R \gg 1$, s.t. $|\Psi(x)| \geq \delta > 0$ for $x : |x| = R$. (Since $\Psi \in H^2_{\text{loc}}(\mathbb{R}^2)$ and $\int (1-|\Psi|^2)^2 dx < \infty$, one can show that such an R exists.) For more on the degree on Sobolev spaces see Ref. [16]. For each such state, we have the quantization of magnetic flux:

$$\int_{\mathbb{R}^2} B(x)dx = 2\pi \deg(\Psi) \in 2\pi\mathbb{Z},$$

which follows from integration by parts (Stokes theorem) and the requirement that $|\Psi(x)| \to 1$ and $|\nabla_A \Psi(x)| \to 0$ as $|x| \to \infty$.

For vortex lattices (see below) the energy is infinite, but the flux quantization still holds for each lattice cell because of gauge-periodic boundary conditions (see below for details).

2.2.4 Homogeneous solutions

The simplest solutions to the Ginzburg–Landau equations (2.1) are the trivial ones corresponding to physically homogeneous states:

1. the perfect superconductor solution, (Ψ_s, A_s), where $\Psi_s \equiv 1$ and $A_s \equiv 0$ (so the magnetic field $\equiv 0$),
2. the normal metal solution, (Ψ_n, A_n), where $\Psi_n \equiv 0$ and A_n corresponds to a constant magnetic field.

(Of course, any gauge transformation of one of these solutions has the same properties.)

We see that the perfect superconductor is a solution only when the magnetic field $B(x)$ is zero. On the other hand, there is a normal solution for any constant magnetic field (to be thought of as determined by applied external magnetic field).

2.2.5 Type I and Type II superconductors

Assuming magnetic fields are weak and consequently neglecting variations of $|\Psi|^2$, we see from the second equation in (2.1) that (in our units) the magnetic field varies on the length scale 1, the *penetration depth*. Furthermore, if the magnetic field in the first equation in (2.1) vanishes, then the order parameter varies on the length scale $\frac{1}{\kappa}$, the *coherence length*.

The two length scales $1/\kappa$ and 1 coincide at $\kappa = 1/\sqrt{2}$. This critical value $\kappa = 1/\sqrt{2}$ separates superconductors into two classes with different properties:

$\kappa < 1/\sqrt{2}$: Type I superconductors—exhibit first-order (discontinuous, finite size nucleation) phase transitions from the non-superconducting state to the superconducting state (essentially, all pure metals);

$\kappa > 1/\sqrt{2}$: Type II superconductors—exhibit second-order (continuous) phase transitions and the formation of vortex lattices (dirty metals and alloys).

An important quantifier of the difference between type I and type II superconductors is the surface tension. As was observed first in Ref. [35], the surface tension at the interface between the normal and superconducting phases changes sign from positive for $\kappa < 1/\sqrt{2}$ to negative for $\kappa > 1/\sqrt{2}$. In detail, consider a flat interface. Assuming the material is uniform in the directions orthogonal to the x_1-axis, becoming normal as $x_1 \to -\infty$ and superconducting as $x_1 \to \infty$. The interface between these phases is the plane $\{x_1 = 0\}$. (By a translation and a rotation, we can always reduce to this case.) Thus we look for a solution depending only on x_1, $(\Psi(x), A(x)) = (\psi(x_1), a(x_1))$, with the magnetic field in the direction of x_3, the vector potential, a, in the direction of x_2, and with the boundary conditions, $\psi(x_1) \to 0$ and $\operatorname{curl} a(x_1) \to h$ as $x_1 \to -\infty$ and $\psi(x_1) \to 1$ and $\operatorname{curl} a(x_1) \to 0$, as $x_1 \to \infty$.

The boundary conditions at $x_1 = -\infty$ and $x_1 = \infty$ are consistent with the equations, if the applied field h satisfies $h = \kappa/\sqrt{2}$. However, in our units, $h_c := \kappa/\sqrt{2}$ is the thermodynamic critical magnetic field, at which the Gibbs free energies of the superconducting and normal phases are equal. (As the problem is one-dimensional, the integration in the functional (2.2) or (2.3) should be taken in the variable $x = x_1$ only, with the energy being interpreted as the energy per unit area of the interface $\{x_1 = 0\}$.) Then, by the definition [35], the surface tension is the surplus of the Gibbs free energy of such a solution compared to the normal (or superconducting) phase at the applied magnetic field h_c,

$$\sigma := \int_{-\infty}^{\infty} \{g_{h_c}(\psi, a) - g_{h_c}(0, a_c)\}\, dx, \tag{2.7}$$

where $g_h(\psi, a) := \frac{1}{2}[|\nabla_a \psi|^2 + \frac{\kappa^2}{2}(|\psi|^2 - 1)^2 + (\operatorname{curl} a - h)^2]$ (see (2.3)) and $\operatorname{curl} a_c = h_c$. It is shown in Ref. [19] that $\sigma > 0$, if $\kappa < 1/\sqrt{2}$ and $\sigma_{\text{surftens}} > 0$, if $\kappa > 1/\sqrt{2}$, with $\sigma = 0$, if $\kappa = 1/\sqrt{2}$.

2.2.6 Self-dual case $\kappa = 1/\sqrt{2}$

In the *self-dual* case $\kappa = 1/\sqrt{2}$ of (2.1), vortices effectively become noninteracting, and there is a rich multi-vortex solution family. Bogomolnyi [14] found the topological energy lower bound

$$\mathcal{E}(\Psi, A)|_{\kappa=1/\sqrt{2}} \geq \pi \, |\deg(\Psi)| \tag{2.8}$$

and showed that this bound is saturated (and hence the Ginzburg–Landau equations are solved) when certain *first-order* equations are satisfied.

2.2.7 Critical magnetic fields

In superconductivity, there are several critical magnetic fields, two of which (the first and the second critical magnetic fields) are of special importance:

h_{c1} is the field at which the first vortex enters the superconducting sample and

h_{c2} is the field at which a mixed state bifurcates from the normal one.

(The critical field h_{c1} is defined by the condition $G(\Psi_s, A_s) = G(\Psi^{(1)}, A^{(1)})$, where (Ψ_s, A_s) is the perfect superconductor solution, defined above, and $(\Psi^{(1)}, A^{(1)})$ is the 1-vortex solution, defined below, while h_{c2}, by the condition that the linearization of the l.h.s. of (2.1) on the normal state (Ψ_n, A_n) has zero eigenvalue. The field h_{c1} depends on Q and is 0 for $Q = \mathbb{R}^2$. Its asymptotics, as $\kappa \to \infty$, was found rigorously in [4, 8]. One can show that $h_{c2} = \kappa^2$.)

For type I superconductors $h_{c1} > h_{c2}$ and for type II superconductors $h_{c1} < h_{c2}$. In the former case, the vortex states have relatively large energies, that is, are metastable, and therefore are of little importance.

For type II superconductors, there are two important regimes to consider: (1) average magnetic fields per unit area, b, are less than but sufficiently close to h_{c2},

$$0 < h_{c2} - b \ll h_{c2} \tag{2.9}$$

and (2) the external (applied) constant magnetic fields, h, are greater than but sufficiently close to h_{c1},

$$0 < h - h_{c1} \ll h_{c1}. \tag{2.10}$$

The reason the first condition involves b, while the second h, is that the first condition comes from the Ginzburg–Landau equations (which do not involve h), while the second from the Ginzburg–Landau Gibbs free energy.

One of the differences between the regimes (2.9) and (2.10) is that $|\Psi|^2$ is small in the first regime (the bifurcation problem) and large in the second one. If a superconductor fills in the entire $\mathbb{R}^2$, then in the second regime, the average magnetic field per unit area, $b \to 0$, as $h \to h_{c1}$.

2.2.8 Time-dependent equations

A number of dynamical versions of the Ginzburg–Landau equations appear in the literature. Here we list the most commonly studied and physically relevant.

Superconductivity. In the leading approximation, the evolution of a superconductor is described by the gradient-flow-type equations for the Ginzburg–Landau energy

$$\begin{cases} \gamma\partial_{t\Phi}\Psi = \Delta_A\Psi + \kappa^2(1-|\Psi|^2)\Psi, \\ \sigma\partial_{t,\Phi}A = -\operatorname{curl}^*\operatorname{curl}A + \operatorname{Im}(\bar{\Psi}\nabla_A\Psi). \end{cases} \tag{2.11}$$

Here Φ is the scalar (electric) potential, γ a complex number, and σ a two-tensor, and $\partial_{t\Phi}$ is the covariant time derivative $\partial_{t,\Phi}(\Psi, A) = ((\partial_t + i\Phi)\Psi, \partial_t A + \nabla\Phi)$. The second equation is Ampère's law, $\operatorname{curl} B = J$, with $J + J_N + J_S$, where $J_N = -\sigma(\partial_t A + \nabla\Phi)$ (using Ohm's law) is the normal current associated to the electrons not having formed Cooper pairs, and $J_S = \operatorname{Im}(\bar{\Psi}\nabla_A\Psi)$, the supercurrent.

These equations are called the *time-dependent Ginzburg–Landau equations* or the *Gorkov–Eliashberg–Schmidt equations* proposed by Schmid [74] and Gorkov and Eliashberg [37] (earlier versions are proposed by Bardeen and Stephen and Anderson, Luttinger and Werthamer).

Particle physics. The time-dependent $U(1)$ Higgs model is described by

$$\begin{aligned} \partial_{t\Phi}^2\Psi &= \Delta_A\Psi + \kappa^2(1-|\Psi|^2)\Psi \\ \partial_t\partial_{t\Phi}A &= -\operatorname{curl}^*\operatorname{curl}A + \operatorname{Im}(\bar{\Psi}\nabla_A\Psi), \end{aligned} \tag{2.12}$$

coupled (covariant) wave equations describing the $U(1)$-gauge Higgs model of elementary particle physics (written here in the *temporal gauge*). Equations (2.12) are sometimes also called the *Maxwell-Higgs equations*.

For the existence results for these two sets of equations see [17, 25].

In what follows, we concentrate on the Gorkov–Eliashberg–Schmidt equations, (2.11) and, for simplicity of notation, we use the gauge, in which the scalar potential, Φ, vanishes, $\Phi = 0$.

2.3 VORTICES

2.3.1 *n*-vortex solutions

A model for a vortex is given, for each degree $n \in \mathbb{Z}$, by a "radially symmetric" (more precisely *equivariant*) solution of the Ginzburg–Landau equations (2.1) of the form

$$\Psi^{(n)}(x) = f_n(r)e^{in\theta} \quad \text{and} \quad A^{(n)}(x) = a_n(r)\nabla(n\theta)\ , \tag{2.13}$$

where (r, θ) are the polar coordinates of $x \in \mathbb{R}^2$. Note that $\deg(\Psi^{(n)}) = n$. The pair $(\Psi^{(n)}, A^{(n)})$ is called the *n-vortex* (*magnetic* or *Abrikosov* in the case of superconductors and *Nielsen–Olesen* or *Nambu string* in the particle physics case). For superconductors, this is a mixed state with the normal phase residing at the point where the vortex vanishes. The existence of such solutions of the Ginzburg–Landau equations was already noticed by Abrikosov [1] and proven in Ref. [11] (For results on symmetry breaking solutions with finite number of vortices and on pinning of vortices see Refs. [61, 89] and [75], respectively.).

Using self-duality, and consequent reduction to a first-order equations, Taubes [84, 85] has showed that for a given degree n, the family of solutions modulo gauge transformations (*moduli space*) is $2|n|$-dimensional, and the $2|n|$ parameters describe the locations of the zeros of the scalar field, that is, the vortex centers. A review of this theory can be found in the book of Jaffe-Taubes [47].

The n-vortex solution exhibits the length scales discussed above. Indeed, the following asymptotics for the field components of the n-vortex (2.13) were established in Ref. [68] (see also Ref. [47]):

$$\begin{aligned} J^{(n)}(x) &= n\beta_n K_1(r)[1+o(e^{-m_\kappa r})]J\hat{x} \\ B^{(n)}(r) &= n\beta_n K_1(r)\left[1-\tfrac{1}{2r}+O\left(\tfrac{1}{r^2}\right)\right] \\ |1-f_n(r)| &\le ce^{-m_\kappa r},\ |f_n'(r)| \le ce^{-m_\kappa r}, \end{aligned} \tag{2.14}$$

as $r := |x| \to \infty$, where $J^{(n)} := \mathrm{Im}(\overline{\Psi^{(n)}}\nabla_{A^{(n)}}\Psi^{(n)})$ is the n-vortex supercurrent, $B^{(n)} := \mathrm{curl}A^{(n)}$ is the n-vortex magnetic field, $\beta_n > 0$ is a constant, and K_1 is the modified Bessel function of order 1 of the second kind. The length scale of $\Psi^{(n)}$ is $1/m_\kappa$. Since $K_1(r)$ behaves like $ce^{-r}/\sqrt{r}$ for large r, we see that the length scale for $J^{(n)}$ and $B^{(n)}$ is 1. (In fact, for $x \neq 0$, $\Psi^{(n)}$ vanishes as $\kappa \to \infty$.)

2.3.2 Stability

We say the n-vortex is *(orbitally) stable*, if for any initial data sufficiently close to the n-vortex (which includes initial momentum field in the (2.12) case), the solution remains, for all time, close to *an element of the orbit of the n-vortex under the symmetry group*. Here "close" can be taken to mean close in the "energy space" Sobolev norm H^1.

Similarly, for *asymptotic stability*, the solution converges, as $t \to \infty$, to an element of the symmetry orbit (i.e., to a spatially-translated, gauge-transformed n-vortex).

We spell out the definition of the latter. We define the manifold, obtained by action of the symmetry group $\mathbb{R}^2 \times H^2(\mathbb{R}^2,\mathbb{R})$ of the vortex on the vortex $u^{(n)} := (\Psi^{(n)}, A^{(n)})$,

$$\mathcal{M}^{(n)} = \{T_h^{\mathrm{trans}} T_\gamma^{\mathrm{gauge}} u^{(n)} : h \in \mathbb{R}^2,\ \gamma \in H^2(\mathbb{R}^2,\mathbb{R})\}.$$

Let dist_{H^1} denote the H^1-distance to this manifold. We say that the vortex $u^{(n)}$ is *asymptotically stable* under H^1-perturbations, if there is $\delta > 0$ s.t. for any initial condition u_0 satisfying $\mathrm{dist}_{H^1}(u_0, \mathcal{M}^{(n)}) \le \delta$ there exists $g(t) := (h(t), \gamma(t)) \in \mathbb{R}^2 \times H^2(\mathbb{R}^2,\mathbb{R})$, s.t. the solution $u(t)$ of the time-dependent equation ((2.11) or (2.12)) satisfies for a first-order operator, F_m, having $2|n|$ zero–modes that can be calculated semi-explicitly. These modes can be thought of as arising from independent relative motions of vortices, and the fact that they are energy-neutral relates to the vanishing of the vortex interaction at $\kappa = 1/2$ [14,92]. Two of the modes arise from translational symmetry, while careful analysis shows that as κ moves above (respectively below) $1/2$, the $2|n|-2$ "extra" modes become unstable (respectively stable) directions.

Technically, it is convenient, on the first step, to effectively remove the (infinite-dimensional subspace of) gauge-symmetry zero modes, by modifying $L^{(n)}$ to make it coercive in the gauge directions—this leaves only the two zero modes arising from translational invariance remaining.

Let $\mathcal{C}$ be the operation of taking the complex conjugate. The results in (fiber) block decomposition of $L^{(n)}$, mentioned above is given in the following.

Theorem 2.2 [41] *1. Let $\mathcal{H}_m := [\mathrm{L}^2_{rad}]^4$ and define $\mathrm{U} : \mathrm{X} \to \mathcal{H}$, where $\mathcal{H} = \bigoplus_{\mathrm{m}\in\mathbf{Z}} \mathcal{H}_m$, so that on smooth compactly supported v it acts by the formula*

$$(Uv)_m(r) = J_m^{-1} \int_0^{2\pi} \chi_m^{-1}(\theta)\rho_n(e^{i\theta})v(x)d\theta.$$

where $\chi_m(\theta)$ are characters of $\mathrm{U}(1)$, that is, all homomorphisms $\mathrm{U}(1) \to \mathrm{U}(1)$ (explicitly we have $\chi_{\mathrm{m}}(\theta) = \mathrm{e}^{im\theta}$) and

$$J_m : \mathcal{H}_m \to e^{i(m+n)\theta}L^2_{\mathrm{rad}} \oplus e^{i(m-n)\theta}L^2_{\mathrm{rad}} \oplus -ie^{i(m-1)\theta}L^2_{\mathrm{rad}} \oplus ie^{i(m+1)\theta}L^2_{\mathrm{rad}}$$

acting in the obvious way. Then U extends uniquely to a unitary operator.

2. Under U the linearized operator around the vortex, $\mathrm{K}^{(\mathrm{n})}_{\#}$, decomposes as

$$UL^{(n)}U^{-1} = \bigoplus_{m\in\mathbf{Z}} L^{(n)}_m, \tag{2.18}$$

where the operators $\mathrm{L}^{(\mathrm{n})}_{\mathrm{m}}$ act on $\mathcal{H}_{\mathrm{m}}$ as $\mathrm{J}^{-1}_{\mathrm{m}}\mathrm{L}^{(\mathrm{n})}\mathrm{J}_{\mathrm{m}}$.

3. The operators $\mathrm{K}^{(\mathrm{n})}_{\mathrm{m}}$ have the following properties:

$$K^{(n)}_m = RK^{(n)}_{-m}R^T, \text{ where } R = \begin{pmatrix} Q & 0 \\ 0 & Q \end{pmatrix}, Q = \begin{pmatrix} 0 & \mathcal{C} \\ \mathcal{C} & 0 \end{pmatrix}, \tag{2.19}$$

$$\sigma_{ess}(K^{(n)}_m) = [\min(1,\lambda), \infty), \tag{2.20}$$

$$\text{for } |n| = 1 \text{ and } m \geq 2,\ L^{(n)}_m - L^{(n)}_1 \geq 0 \text{ with no zero-eigenvalue}, \tag{2.21}$$

$$L^{(n)}_0 \geq c > 0 \quad \text{for all } \kappa, \tag{2.22}$$

$$L^{(\pm 1)}_1 \geq 0 \text{ with non-degenerate zero-mode given by (2.17)}. \tag{2.23}$$

Since by (2.20) and (2.23), $L_1^{(\pm 1)}|_{T^\perp} \geq \tilde{c} > 0$ and, by (2.22) and (2.23), $L_m^{(\pm 1)} \geq c' > 0$ for $|m| \geq 2$, this theorem implies (2.15).

2.4 VORTEX LATTICES

In this section, we describe briefly recent results on vortex lattice solutions, that is solutions that display vortices arranged along vertices of a lattice in $\mathbb{R}^2$. Since their discovery by Abrikosov in 1957, solutions have been studied in numerous experimental and theoretical works (of the more mathematical studies, we mention the articles of Eilenberger [30] and Lasher [53]).

The rigorous investigation of Abrikosov solutions was carried out by Odeh [58], soon after their discovery. Odeh has given a detailed sketch of the proof of the bifurcation of Abrikosov solutions at the second critical magnetic field. Further details were provided by Barany, Golubitsky, and Tursky [9], using equivariant bifurcation theory, and by Takáč [83], who obtained results on the zeros of the bifurcating solutions. The proof of existence was completed by Tzneteas and Sigal [89] and extended further by Tzaneteas and Sigal [90] beyond the cases covered in the works above.

Existence of Abrikosov solutions at low magnetic fields near the first critical magnetic field was given in Ref. [76].

Moreover, Odeh has also given a detailed sketch of the proof, with details in Ref. [29], of the existence of Abrikosov solutions using the variational minimization of the Ginzburg–Landau energy functional reduced to a fundamental cell of the underlying lattice. However, this proof provides only very limited information about the solutions.

Chapman [20] and Almag [6] gave a detailed analysis of extension of Abrikosov solutions to higher magnetic fluxes per fundamental cells.

Moreover, important and fairly detailed results on asymptotic behavior of solutions, for $\kappa \to \infty$ and the applied magnetic fields, h, satisfying $h \leq \frac{1}{2} \log \kappa + \text{const}$ (the London limit), were obtained by Aydi and Sandier [8] (see Ref. [71] for references to earlier works). Further extensions to the Ginzburg–Landau equations for anisotropic and high-temperature superconductors can be found in Refs. [4, 5].

Among related results, a relation of the Ginzburg–Landau minimization problem, for a fixed, finite domain and in the regime of the Ginzburg–Landau parameter $\kappa \to \infty$ and external magnetic field, to the Abrikosov lattice variational problem was obtained Ref. [3] (see also Ref. [7]). Dutour [28] (see also Ref. [29]) has found boundaries between superconducting, normal, and mixed phases. In Ref. [7, 8], the Ginzburg–Landau energy is connected to the thermodynamic limit of the Abrikosov energy. The complete proof of the thermodynamic limit of the Abrikosov energy is given in Ref. [33] and boundary effects on the Abrikosov energy are established in Ref. [32]. The connection between vortex lattice problems and the Ginzburg–Landau functional is established in the large kappa limit in Ref. [72].

The proof that the triangular lattices minimize the Ginzburg–Landau energy functional per the fundamental cell was obtained in [89]. The paper used original Abrikosov ideas and the results of [2, 56] on the Abrikosov "constant".

The stability of Abrikosov lattices is shown in Ref. [77] for gauge periodic perturbations, that is, perturbations having the same translational lattice symmetry as the solutions themselves, and in Ref. [78] for local, more precisely, H^1, perturbations.

Here we describe briefly the existence and stability results and the main ideas entering into their proofs.

2.4.1 Abrikosov lattices

In 1957, A. Abrikosov [1] discovered a class of solutions, (Ψ, A), to (2.1), presently known as Abrikosov lattice vortex states (or just Abrikosov lattices), whose physical characteristics, density of Cooper pairs, $|\Psi|^2$, the magnetic field, $\mathrm{curl}A$, and the supercurrent, $J_S = \mathrm{Im}(\bar{\Psi}\nabla_A \Psi)$, are double-periodic w.r.t a lattice $\mathcal{L}$. (This set of states is invariant under the symmetries of the previous subsection.)

For Abrikosov states, for (Ψ, A), the magnetic flux, $\int_\Omega \mathrm{curl}A$, through a fundamental lattice cell, Ω, is quantized,

$$\frac{1}{2\pi}\int_\Omega \mathrm{curl}A = \deg \Psi = n, \tag{2.24}$$

for some integer n. Indeed, the periodicity of $n_s = |\Psi|^2$ and $J = \mathrm{Im}(\bar{\Psi}\nabla_A \Psi)$ implies that $\nabla\varphi - A$, where $\Psi = |\Psi|e^{i\varphi}$, is periodic, provided $\Psi \neq 0$ on $\partial\Omega$. This, together with Stokes's theorem, $\int_\Omega \mathrm{curl}A = \oint_{\partial\Omega} A = \oint_{\partial\Omega} \nabla\varphi$ and the single-valuedness of Ψ, implies that $\int_\Omega \mathrm{curl}A = 2\pi n$ for some integer n. Using the reflection symmetry of the problem, one can easily check that we can always assume $n \geq 0$.

Equation (2.24) implies the relation between the average magnetic flux, b, per lattice cell, $b = 1/|\Omega|\int_\Omega \mathrm{curl}A$, and the area, $|\Omega|$, of a fundamental cell

$$b = \frac{2\pi n}{|\Omega|}. \tag{2.25}$$

Finally, it is clear that the gauge, translation, and rotation symmetries of the Ginzburg–Landau equations map lattice states to lattice states. In the case of the gauge and translation symmetries, the lattice with respect to which the solution is gauge-periodic does not change, whereas with the rotation symmetry, the lattice is rotated as well. The magnetic flux per cell of solutions is also preserved under the action of these symmetries.

2.4.2 Existence of Abrikosov lattices

We assume always that the coordinate origin is placed at one of the vertices of the lattice $\mathcal{L}$. Recall that we identify $\mathbb{R}^2$ with $\mathbb{C}$, via the map $(x_1, x_2) \to x_1 + ix_2$. We can choose a basis in $\mathcal{L}$ so that $\mathcal{L} = r(\mathbb{Z} + \tau\mathbb{Z})$, where $\tau \in \mathbb{C}$, $\mathrm{Im}\,\tau > 0$, and $r > 0$, with bases giving the same lattice related by elements of the modular group $SL(2, \mathbb{Z})$ (see Appendix 2.A for details). Hence, it suffices to consider τ in the fundamental domain,

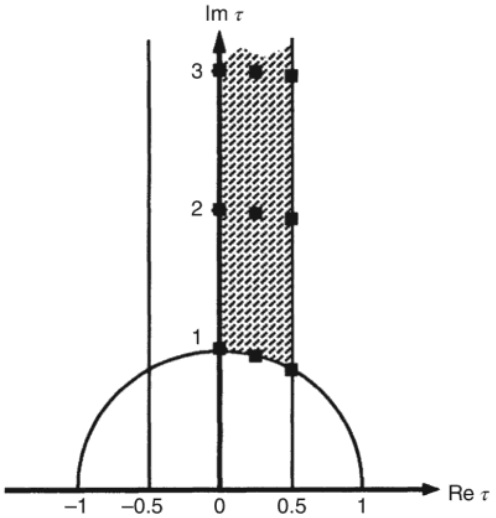

FIGURE 2.1 Half of the fundamental domain $\Pi^+/SL(2,\mathbb{Z})$.

$\Pi^+/SL(2,\mathbb{Z})$, of $SL(2,\mathbb{Z})$ acting on the Poincaré half-plane $\Pi^+ := \{\tau \in \mathbb{C} : \operatorname{Im}\tau > 0\}$ (see Fig. 2.1).

Due to the quantization relation (2.25), the parameters τ, b, and n determine the lattice $\mathcal{L}$ up to a rotation and a translation. As the equations (2.1) are invariant under rotations and translations, solutions corresponding to translated and rotated lattices are related by symmetry transformations and therefore can be considered equivalent, with equivalence classes determined by triples $\omega = (\tau, b, n)$, specifying the underlying lattice has shape τ, the average magnetic flux per lattice cell b, and the number n of quanta of magnetic flux per lattice cell. With this in mind, we will say that an Abrikosov lattice state (Ψ, A) is of type $\omega = (\tau, b, n)$, if it belongs to the equivalence class determined by $\omega = (\tau, b, n)$.

Let $\beta(\tau)$ be the Abrikosov "constant," defined in (2.33) below. The following critical value of the Ginzburg–Landau parameter κ plays an important role in what follows

$$\kappa_c(\tau) := \sqrt{\frac{1}{2}\left(1 - \frac{1}{\beta(\tau)}\right)}. \tag{2.26}$$

Recall that the value of the second critical magnetic field at which the normal material undergoes the transition to the superconducting state is that $h_{c2} = \kappa^2$.

For the case $n = 1$ of one quantum of flux per unit cell, the following result establishes the existence of nontrivial lattice solutions near the normal metal solution:

Theorem 2.3 [9, 29, 58, 90] *Fix a lattice shape* τ *and let* b *satisfy*

$$|\kappa^2 - b| \ll \kappa^2[(2\kappa^2-1)\beta(\tau)+1] \tag{2.27}$$

(uniformly in the parameters τ *and* b*) and*

$$\text{either } \kappa > \kappa_c(\tau),\ \kappa^2 > b \ \text{ or } \ \kappa < \kappa_c(\tau),\ \kappa^2 < b. \tag{2.28}$$

Then for $\omega = (\tau, b, 1)$

- *there exists a smooth Abrikosov lattice solution* $u_\omega = (\Psi_\omega, A_\omega)$ *of type* ω.

Remark. For $\kappa > 1/\sqrt{2}$ and the triangular and square lattices the theorem was proven in Refs. [9, 29, 58, 89], and in the case stated in Refs. [89, 90].

Let $\mathcal{L}_\omega$ be the lattice specified by a triple $\omega = (\tau, b, n)$ and let Ω_ω denote its elementary cell. Define the average energy, $E_b(\tau) := \frac{1}{|\Omega_\omega|}\mathcal{E}_{\Omega_\omega}(u_\omega)$, per lattice cell, of the Abrikosov lattice solution, u_ω, $\omega = (\tau, b, 1)$, found in Theorem 2.3.

Theorem 2.4 [90] *Let* $\kappa > 1/\sqrt{2}$ *and let b satisfy* $b < \kappa^2$ *and* (2.27). *Then for a fixed* b,

- $E_b(\tau)$ *has the global minimum in* τ *at the hexagonal (equilateral triangular) lattice,* $\tau = e^{i\pi/3}$.

(Due to a calculation error, Abrikosov concluded that the lattice that gives the minimum energy is the square lattice. The error was corrected by Kleiner et al. [51], who showed that it is in fact the triangular lattice that minimizes the energy.)

Now, we formulate the existence result for low magnetic fields, those near the first critical magnetic field h_{c1}: Let $\mathcal{L}_\omega$ be a lattice specified by a triple $\omega = (\tau, b, n)$ and let Ω_ω denote its elementary cell. We have the following.

Theorem 2.5 [76] *Let* $\kappa \neq 1/\sqrt{2}$ *and fix a lattice shape* λ *and* $\mathrm{n} \neq 0$. *Then there is* $\mathrm{b}_0 = \mathrm{b}_0(\kappa)$ $(\sim (\kappa - 1/\sqrt{2})^2) > 0$ *such that for* $\mathrm{b} \leq \mathrm{b}_0$, *there exists an odd solution Abrikosov lattice solution* $\mathrm{u}_\omega \equiv (\Psi_\omega, \mathrm{A}_\omega)$ *of* (2.1), *s.t.*

$$u_\omega(x) = u^{(n)}(x-\alpha) + O(e^{-c\rho}) \ \text{ on } \ \Omega_\omega + \alpha,\ \forall \alpha \in \mathcal{L}_\omega, \tag{2.29}$$

where $u^{(n)} := (\Psi^{(n)}, \mathrm{A}^{(n)})$ *is the n-vortex,* $\rho = \mathrm{b}^{-1/2}$, *and* $c > 0$, *in the sense of the local Sobolev norm of any index.*

In the next two subsections, we present a discussion of some key general notions. After this, we outline the proofs of the results above.

where g_s satisfies (2.31). By (2.32), it can be taken to be

$$g_s(x) = \frac{b}{2} s \wedge x + c_s, \tag{2.36}$$

where b is the average magnetic flux, $b = 1/|\Omega| \int_\Omega \operatorname{curl} A$ (satisfying (2.25) so that $bs \wedge t \in 2\pi\mathbb{Z}$), and c_s satisfies

$$c_{s+t} - c_s - c_t - \frac{1}{2} bs \wedge t \in 2\pi\mathbb{Z}. \tag{2.37}$$

The linearized problem. We expect that as the average flux b decreases below $h_{c2} = \kappa^2$, a vortex lattice solution emerges from the normal material solution (Ψ_n, A_n), where $\Psi_n = 0$ and A_n is a magnetic potential, with the constant magnetic field b. Note that $(\Psi_n, A_n) = (0, A^b)$ satisfies (2.35), if we take the gauge $A^b = (-b/2)Jx$. Linearizing (2.1) at $(0, A^b)$ leads to the linearized problem

$$(-\Delta_{A^b} - \kappa^2)\phi = 0, \tag{2.38}$$

with $\phi(x)$ satisfying

$$\phi(x+s) = e^{i\frac{b}{2} s \cdot Jx} \phi(x), \quad \forall s \in \mathcal{L}. \tag{2.39}$$

(The second equation in (2.1) leads to $\operatorname{curl} a = 0$ which gives, modulo gauge transformation, $a = 0$.) We show that this problem has n linearly independent solutions, provided $b|\Omega| = 2\pi n$ and $b = \kappa^2 = h_{c2}$.

Denote by L^b the operator $-\Delta_{A^b}$, defined on the lattice cell Ω with the lattice boundary conditions in (2.39), is self-adjoint, has a purely discrete spectrum, and evidently satisfies $L^b \geq 0$. We have the following well-known result

Proposition 2.1 *The operator L^b is self-adjoint, with the purely discrete spectrum given by the spectrum explicitly as*

$$\sigma(L^b) = \{ (2k+1)b : k = 0, 1, 2, \dots, \}, \tag{2.40}$$

and each eigenvalue is of the same multiplicity.

If $b|\Omega| = 2\pi n$, then this multiplicity is n and, in particular, we have

$$\dim_{\mathbb{C}} \operatorname{Null}(L^b - b) = n.$$

Proof: The self-adjointness is standard. Spectral information about L^b can be obtained by introducing the complexified covariant derivatives (harmonic oscillator annihilation and creation operators), $\bar{\partial}_{A^b}$ and $\bar{\partial}^*_{A^b} = -\partial_{A^b}$, with

$$\bar{\partial}_{A^b} := (\nabla_{A^b})_1 + i(\nabla_{A^b})_2 = \partial_{x_1} + i\partial_{x_2} + \frac{1}{2} bx_1 + \frac{1}{2} ibx_2. \tag{2.41}$$

One can verify that these operators satisfy the following relations:

1. $[\bar{\partial}_{A^b}, \bar{\partial}^*_{A^b}] = 2\,\mathrm{curl} A^b = 2b$;
2. $-\Delta_{A^b} - b = \bar{\partial}^*_{A^b}\bar{\partial}_{A^b}$.

As for the harmonic oscillator (see e.g., Ref. [42]), this gives the spectrum explicitly (2.40). This proves the first part of the theorem.

For the second part, a simple calculation gives the following operator equation

$$e^{\frac{b}{2}(ix_1x_2 - x_2^2)}\bar{\partial}_{A^b}e^{-\frac{b}{2}(ix_1x_2 - x_2^2)} = \partial_{x_1} + i\partial_{x_2}.$$

This immediately proves that $\Psi \in \mathrm{Null}\,\bar{\partial}_{A^b}$ if and only if $\xi(x) = e^{\frac{b}{2}(ix_1x_2 - x_2^2)}\psi(x)$ satisfies $\partial_{x_1}\xi + i\partial_{x_2}\xi = 0$.

We identify $\mathbb{R}^2$ with $\mathbb{C}$, via the map $(x_1, x_2) \to x_1 + ix_2$. We can choose a basis in $\mathcal{L}$ so that $\mathcal{L} = r(\mathbb{Z} + \tau\mathbb{Z})$, where $\tau \in \mathbb{C}$, $\mathrm{Im}\,\tau > 0$, and $r > 0$. By the quantization condition (2.25), $r := \sqrt{\frac{2\pi n}{\mathrm{Im}\,\tau b}}$. Define $z = \frac{1}{r}(x_1 + ix_2)$ and

$$\theta(z) = e^{\frac{b}{2}(ix_1x_2 - x_2^2)}\phi(x). \tag{2.42}$$

By the above, the function θ is entire and, due to the periodicity conditions on ϕ, satisfies

$$\theta(z+1) = \theta(z),$$
$$\theta(z+\tau) = e^{-2inz}e^{-in\tau z}\theta(z).$$

Hence θ is the theta function. By the first relation, θ has the absolutely convergent Fourier expansion

$$\theta(z) = \sum_{k=-\infty}^{\infty} c_k e^{2\pi kiz}. \tag{2.44}$$

with the coefficients satisfying $c_{k+n} = e^{in\pi\tau}e^{2ki\pi\tau}c_k$, which means such functions are determined by $c_0, \dots, c_{n-1}$ and therefore form an n-dimensional vector space. This proves Proposition 2.1.

This also gives the form of the leading approximation (2.42)–(2.44) to the true solution.

The nonlinear problem. Now let $n = 1$. Once the linearized map is well understood, it is possible to construct solutions, u_ω, $\omega = (\tau, b, 1)$, of the Ginzburg–Landau equations for a given lattice shape parameter τ, and the average magnetic flux b near h_{c2}, via a Lyapunov–Schmidt reduction.

Comments on the proof of Theorem 2.4 The relation between the Abrikosov function and the average energy, $E_b(\tau) := \frac{1}{|\Omega_\omega|}\mathcal{E}_{\Omega_\omega}(u_\omega)$, of this solution is given by the following result (see Ref. [89]).

Proposition 2.2 *In the case $\kappa > \frac{1}{\sqrt{2}}$, the minimizers, τ_b, of $\tau \mapsto E_b(\tau)$ are related to the minimizer, τ_*, of $\beta(\tau)$, as $\tau_b - \tau_* = O(\mu^{1/2})$. In particular, $\tau_b \to \tau_*$ as $b \to \kappa^2$.*

This result was already found (non-rigorously) by Abrikosov [1]. Thus the problem of minimization of the energy per the lattice cell is reduced to finding the minima of $\beta(\tau)$ as a function of the lattice shape parameter τ.

Using symmetries of $\beta(\tau)$, one can also show (see Ref. [78] and remark after Theorem 2.8) that $\beta(\tau)$ has critical points at the points $\tau = e^{\pi i/3}$ and $\tau = e^{\pi i/2}$. However, to determine minimizers of $\beta(\tau)$ requires a rather delicate analysis, which gives the following.

Theorem 2.6 [2,57] *The function $\beta(\tau)$ has exactly two critical points, $\tau = e^{i\pi/3}$ and $\tau = e^{i\pi/2}$. The first is minimum, while the second is a maximum.*

Hence the second part of Theorem 2.4 follows.

Comments on the proof of Theorem 2.5. The idea here is to reduce solving (2.1) for (Ψ, A) on the space $\mathbb{R}^2$ to solving it for (ψ, a) on the fundamental cell Ω, satisfying the boundary conditions

$$\begin{cases} \psi(x+s) = e^{ig_s(x)}\psi(x), \\ a(x+s) = a(x) + \nabla g_s(x), \\ (\nu \cdot \nabla_a \psi)(x+s) = e^{ig_s(x)}(\nu \cdot \nabla_a \psi)(x), \\ \operatorname{curl} a(x+s) = \operatorname{curl} a(x), \\ x \in \partial_1\Omega/\partial_2\Omega \text{ and } s = \omega_1/\omega_2. \end{cases} \tag{2.45}$$

induced by the periodicity condition (2.35). Here $\partial_1\Omega/\partial_2\Omega =$ the left/bottom boundary of Ω, $\{\omega_1, \omega_2\}$ is a basis in $\mathcal{L}$ and $\nu(x)$ is the normal to the boundary at x.

To this end we show that given a continuously differentiable function (ψ, a) on the fundamental cell Ω, satisfying the boundary conditions (2.45), with g_s satisfying (2.31), we can lift it to a continuous and continuously differentiable function (Ψ, A) on the space $\mathbb{R}^2$, satisfying the gauge-periodicity conditions (2.35). Indeed, we define for any $\alpha \in \mathcal{L}$,

$$\Psi(x) = \psi(x-\alpha)e^{i\Phi_\alpha(x)},\ A(x) = a(x-\alpha) + \nabla\Phi_\alpha(x),\ x \in \Omega + \alpha, \tag{2.46}$$

where $\Phi_\alpha(x)$ is a real, possibly multi-valued, function to be determined. (Of course, we can add to it any $\mathcal{L}-$periodic function.) We define

$$\Phi_\alpha(x) := g_\alpha(x-\alpha),\ \text{for } x \in \Omega + \alpha. \tag{2.47}$$

Lemma. Assume functions (ψ, a) on Ω are twice differentiable, up to the boundary, and obey the boundary conditions (2.45) and the Ginzburg–Landau equations (2.1). Then the functions (Ψ, A), constructed in (2.46) and (2.47), are smooth in $\mathbb{R}^2$ and satisfy the periodicity conditions (2.35) and the Ginzburg–Landau equations (2.1).

Proof: If (ψ, a) satisfies the Ginzburg–Landau equations (2.1) in Ω, then $U \equiv (\Psi, A)$, constructed in (2.46) and (2.47), has the following properties

(1) (Ψ, A) is twice differentiable and satisfies (2.1) in $\mathbb{R}^2/(\cup_{t\in\mathcal{L}} S_t \partial\Omega)$, where $S_t : x \to x+t$;
(2) (Ψ, A) is continuous with continuous derivatives ($\nabla_A \Psi$ and $\operatorname{curl} A$) in $\mathbb{R}^2$ and satisfies the gauge-periodicity conditions (2.35) in $\mathbb{R}^2$.

Indeed, the periodicity condition (2.35) applied to the cells $\Omega + \alpha - \omega_i$ and $\Omega + \alpha$ and the continuity condition on the common boundary of the cells $\Omega + \alpha - \omega_i$ and $\Omega + \alpha$ imply that $\Phi_\alpha(x)$ should satisfy the following two conditions:

$$\Phi_\alpha(x) = \Phi_{\alpha-\omega_i}(x-\omega_i) + g_{\omega_i}(x-\omega_i), \text{ mod } 2\pi, \; x \in \Omega + \alpha, \tag{2.48}$$

$$\Phi_\alpha(x) = \Phi_{\alpha-\omega_i}(x) + g_{\omega_i}(x-\alpha), \text{ mod } 2\pi, \; x \in \partial_i\Omega + \alpha, \tag{2.49}$$

where $i = 1, 2$, and, recall, $\{\omega_1, \omega_2\}$ is a basis in $\mathcal{L}$ and $\partial_1\Omega/\partial_2\Omega$ is the left/bottom boundary of Ω.

To show that (2.47) satisfies the conditions (2.48) and (2.49), we note that, due to (2.31), we have $g_\alpha(x-\alpha) = g_{\alpha-\omega_i}(x-\alpha) + g_{\omega_i}(x-\omega_i)$, mod 2π, $x \in \Omega + \alpha$, and $g_\alpha(x-\alpha) = g_{\alpha-\omega_i}(x-\alpha+\omega_i) + g_{\omega_i}(x-\alpha)$, mod 2π, $x \in \partial_i\Omega + \alpha$, which are equivalent to (2.48) and (2.49), with (2.47).

The second pair of conditions in (2.45) implies that $\nabla_A \Psi$ and $\operatorname{curl} A$ are continuous across the cell boundaries.

By (1) and (2), the derivatives $\Delta_A \Psi$ and $\operatorname{curl}^2 A$ are continuous, up to the boundary, in $S_t \partial\Omega$, for every $t \in \mathcal{L}$. By (2.1), they are equal in $\mathbb{R}^2/(\cup_{t\in\mathcal{L}} S_t \partial\Omega)$ to functions continuous in $\mathbb{R}^2$ satisfying there the periodicity condition (2.35). Hence, they are also continuous and satisfy the periodicity condition (2.35) in $\mathbb{R}^2$. By iteration of the above argument (i.e., elliptic regularity), Ψ, A are smooth functions obeying (2.35) and (2.1).

Now, we use the $n-$vortex $(\Psi^{(n)}, A^{(n)})$, placed in the center of the fundamental cell Ω, to construct an approximate solution $(\psi^{\text{appr}}, a^{\text{appr}})$ to (2.1) in Ω, satisfying (2.45), and use it and the Lyapunov–Schmidt splitting technique to show that there is a true solution (ψ, a) nearby sharing the same properties. After that, we use Lemma 2.4.5 above to lift (ψ, a) to a solution (Ψ, A) on the space $\mathbb{R}^2$, satisfying the gauge-periodicity conditions (2.35).