Interdisciplinary Applied Mathematics

Volume 33

Problems in engineering, computational science, and the physical and biological sciences are using increasingly sophisticated mathematical techniques. Thus, the bridge between the mathematical sciences and other disciplines is heavily traveled. The correspondingly increased dialog between the disciplines has led to the establishment of the series: *Interdisciplinary Applied Mathematics*.

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The series will consist of monographs and high-level texts from researchers working on the interplay between mathematics and other fields of science and technology.

Interdisciplinary Applied Mathematics

Volumes published are listed at the end of the book

Marco Pettini

Geometry and Topology in Hamiltonian Dynamics and Statistical Mechanics

Springer

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To the memory of my father

Foreword

It is a special pleasure for me to write this foreword for a remarkable book by a remarkable author. Marco Pettini is a deep thinker, who has spent many years probing the foundations of Hamiltonian chaos and statistical mechanics, in particular phase transitions, from the point of view of geometry and topology.

It is in particular the quality of mind of the author and his deep physical, as well as mathematical insights which make this book so special and inspiring. It is a "must" for those who want to venture into a new approach to old problems or want to use new tools for new problems.

Although topology has penetrated a number of fields of physics, a broad participation of topology in the clarification and progress of fundamental problems in the above-mentioned fields has been lacking. The new perspectives topology gives to the above-mentioned problems are bound to help in their clarification and to spread to other fields of science.

The sparsity of geometric thinking and of its use to solve fundamental problems, when compared with purely analytical methods in physics, could be relieved and made highly productive using the material discussed in this book.

It is unavoidable that the physicist reader may have then to learn some new mathematics and be challenged to a new way of thinking, but with the author as a guide, he is assured of the best help in achieving this that is presently available.

The major mathematical tool used by the author to tackle the problems mentioned in the title is Riemannian differential geometry, the same as is used in general relativity. This way a geometric based theory of Hamiltonian chaos and thermodynamic phase transitions is pursued. Moreover, a connection is made between the origin of Hamiltonian chaos and phase transitions. In this approach the origin of both is related to curvature fluctuations of the phase space of the system.

I note that for the mathematically inclined reader the use of a coordinate-dependent formulation based on Riemannian geometry may be less satisfactory than for the physicist reader and might be considered a lack of mathematical elegance. After all, geometry's and topology's virtue is a global approach to the structure of manifolds and their properties. However, from a physicist's point of view one might invoke Boltzmann's dictum that "elegance is for tailors."

The above-mentioned curvature variations in the Riemannian description of phase space lead then, on the one hand, to Hamiltonian chaos through a parametric instability mechanism. On the other hand, when they are also due to the additional cause of a strongly and suddenly changing complex topology, they are also closely related to phase transitions. In fact, numerical studies show that a phase transition is invariably marked by a peak in the curvature fluctuations and by "cuspy" energy dependencies of Lyapunov exponents.

Thus these catastrophic events, due to the highly irregular, "bumpy" landscape of phase space, trigger on the deeper level of the topology of phase space itself the singularities occurring in the usual description of phase transitions on a higher level.

A remarkable achievement is the proof of two theorems, giving, for a large class of Hamiltonian systems, a necessary topological condition for a first- or second-order phase transition to take place. Roughly speaking, these theorems say, "no topology change in phase space, no phase transition." However, there is at present no theorem that gives a sufficient topological condition for the occurrence of a phase transition.

This may be related to the fact that not every topological transition in phase space leads to a phase transition, so that the question arises, what kinds of topological transitions are related to phase transitions and what is, from a topological point of view, the difference between various types of phase transitions?

Clearly the elucidation of these questions would deepen our basic understanding of two of the most striking phenomena in nature: that of chaos and that of phase transitions.

It is my conviction that this book makes a courageous attempt to clarify these fundamental phenomena in a new way.

Therefore, I highly recommend this refreshing and very original book not only for its factual content but also for the privilege one has in sharing the author's deep insights and new approaches and results to some unsolved problems in physics. I have no doubt that the reader will find this book highly stimulating and rewarding.

E. G. D. Cohen, professor
The Rockefeller University
New York, July 2006

Preface

Phase transitions are among the most impressive phenomena occurring in nature. They are an example of *emergent* behavior, i.e., of collective properties having no direct counterpart in the dynamics or structure of individual atoms or molecules: to give a familiar example, the molecules of ice and liquid water are identical and interact with the same laws of force, despite their remarkably different macroscopic properties.

That these macroscopic properties must have some relation to microscopic dynamics seems obvious, for example the molecules in a drop of water are free to move everywhere in the drop, in contrast to what happens in a crystal of ice.

However, according to a widespread point of view, when a large number of particles is involved, since we are unable to follow all their individual histories, we are compelled to get rid of dynamics and to replace it by a statistical description. For a long time only a marginal role has been thus attributed to microscopic dynamics: the large number of particles and our ignorance of their initial conditions have been considered enough to provide a solid ground to statistical mechanics.

More recently, much attention has been paid to another source of unpredictability, which is intrinsic to the dynamics itself: deterministic chaos, and, in particular, Hamiltonian chaos.

The present book is a monograph committed to a synthesis of two basic topics in physics: Hamiltonian dynamics, with all its richness unveiled since the famous numerical experiment of Fermi and coworkers at Los Alamos, and statistical mechanics, mainly for what concerns phase transition phenomena in systems described by realistic interatomic or intermolecular forces.

The novelty of the theoretical proposal put forward in this monograph stems from a well-known fact: the natural motions of a Hamiltonian system are geodesics of appropriately defined Riemannian manifolds. Whence the possibility of deepening our understanding of the microscopic dynamical foundations of macroscopic physics of many-particle systems. In fact, the geometrization of dynamics allows questions like, can we “read” in the geometry of these mechanical manifolds something relevant to the understanding of basic properties of the dynamics? A major issue is undoubtely to understand the origin of the chaotic instability of dynamics. The first part of the book contains what we can call the beginning of a Riemannian theory of Hamiltonian chaos, which works strikingly well when applied to models (like the Fermi–Pasta–Ulam model) fulfilling the simplifying hypotheses introduced to analytically compute the largest Lyapunov exponent. In the spirit of the Springer Series in Interdisciplinary Applied Mathematics, I have made explicit in what direction further developments of the theory should go. The second part of the book stems from another question, again rooted in the Riemannian theory of chaos: what happens to these mechanical manifolds when a Hamiltonian system undergoes a phase transition? and how can we "geometrically read" the occurrence of a phase transition? It is at this point that topology comes into play, and, roughly speaking, considering certain submanifolds of configuration space, the answer is that necessarily a phase transition can occur only at a point where the topology of these submanifolds undergoes a transition, and this is true at least for a large class of systems.

The presentation of the book follows the logic of the historical development of a successful ten-year research program that I carried out with the help of several collaborators. The many open points are at the same time highlighted, giving the material presented more the form of an intermediate stage of publication than the form of a monograph on a mature and already concluded research program. And it is just this characteristic that, I hope, will make this book attractive for those, mathematicians or physicists, who might be interested in contributing to the general theoretical framework, its physical applications, or the mathematics necessary in the context of applications.

The mathematics involved is not used to clean up or rephrase already existing results, rather it is constructively used to gain insight. The language of differential geometry and differential topology is not familiar to the majority of physicists and has almost never entered statistical mechanics, a circumstance that might induce skepticism and/or could be discouraging.

Thus, in order to make this book accessible to as wide a readership as possible, including both mathematicians and physicists, and since it makes use of concepts that might be not known to everyone, the following format has been chosen.

The first part of the book is aimed at a reader who is familiar with the basics of Riemannian geometry, for example at the level of a course in general relativity. As to the second part, a knowledge of Morse theory and de Rham's cohomology theory at an elementary level is assumed. However, for those physicists who are not familiar with these branches of mathematics, I have provided in appendices the main points that are needed to follow the exposition. Similarly, I assume that the reader is familiar with the basics of Hamiltonian dynamical systems (theory and phenomenology) and statistical mechanics, but I have summarized in Chapter 2 the main concepts needed throughout the book. In all cases references to the literature for the details are made. I hope that a reader familiar with the basic mathematical tools and with the basic physical meaning of the topics treated will be able to read the book straightforwardly.

I have made a special effort to emphasize logical coherence and the excellent consistency already attained by the ensemble of results presented in the book. Nevertheless, as mentioned above, these results constitute the starting of a new theory rather than its completion. This is the reason why this monograph has no pretence at mathematical rigor (with the exception of Chapter 9), nor at mathematical elegance (the geometrization of Hamiltonian flows, their integrability and instability, in Chapters 3, 4, and 5, respectively, is written in a coordinate-dependent style in view of applications and thus of explicit computations). Nevertheless, I hope that this will not prevent mathematicians from understanding the meaning of what has been achieved in applying geometrical and topological methods to the study of the relationship between dynamical systems and statistical mechanics, with special emphasis on phase transitions. In fact, I would like this monograph to allow the reader, mathematician or physicist, to familiarize herself or himself with this new field and to stimulate new developments and contributions to the many points that are still open and explicitly evidenced throughout the text.

The theoretical scenario depicted in this book is based on the outcomes of a research program inspired and coordinated by the author. However, this research program has been successfully developed only thanks to the collective effort of several collaborators and friends. Therefore, among the most senior of them, my warmest thanks go to Monica Cerruti-Sola, whose continual and precious collaboration during fifteen years has been of invaluable help. My warmest acknowledgments also go to Giulio Pettini for having contributed during a crucial period. I have been honored by the active interest in this research program demonstrated by E.G.D. Cohen and Raoul Gatto, with whom stimulating and fruitful collaborations were carried on during several years.

At the very beginning of my interest in the connection between Hamiltonian dynamics and statistical mechanics, there was a collaboration, a long time ago, with Roberto Livi, Antonio Politi, Stefano Ruffo, and Angelo Vulpiani, friends and colleagues with whom useful discussions and scientific interchanges have never ceased.

I had the chance to work with several gifted and very brilliant PhD students. Among them, my warmest acknowledgments go to Lapo Casetti, who has creatively, brilliantly, and courageously contributed to most of the fundamental steps of this research program since its very beginning; as well, my warmest acknowledgments go to Roberto Franzosi, whose brilliant, creative, and continual collaboration during the last ten years has been of invaluable help in making crucial leaps forward in the topological theory of phase transitions.

It is with a feeling of deepest sorrow that my memory goes to another student and dear friend of mine, Lando Caiani, who died while he was at

SISSA-ISAS in Trieste for his PhD. Lando was an outstanding, very promising, and cultivated young physicist.

A precious contribution to the Riemannian approach to the study of Hamiltonian chaos and to the early developments of the topological approach to phase transitions was given by Cecilia Clementi, whose intelligence and productivity were nothing but absolutely impressive.

It is a pleasure to acknowledge the precious help of Lionel Spinelli in working out rigorous results on the topological theory of phase transitions, of Guglielmo Iacomelli, with whom we worked on extensions of these methods to quantum systems, and of Guido Ciraolo, with whom we worked on the Riemannian theory of Hamiltonian chaos of low-dimensional systems.

A timely and very fruitful collaboration with Luca Angelani, Giancarlo Ruocco, and Francesco Zamponi is warmly acknowledged.

I have profited from many helpful discussions about mathematics with Gabriele Vezzosi, whose friendly and continuous interest for this work has been an effective encouragement.

I warmly thank another friend, A.M. Vinogradov, for many illuminating discussions on several topics in mathematics.

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While writing this book I have been supported in many ways by my beloved children Eleonora and Leonardo.

Last, but not least, this book would have not seen the light of day without the invaluable help of Massimo Fagioli, psychiatrist and eminent scientist, who, having unveiled fundamental dynamical processes of the unconscious mind, in Rome has been conducting, since 32 years, the so-called *Analisi Collettiva*, a very large group in which an emergent phenomenon (as in the case of phase transitions!), due to the unconscious interactions among people, has a strong healing power. In this way Massimo Fagioli drew me out of what T.S. Eliot would have called a “waste land,” where I was wandering after my father’s passing away.

Florence, September 2006 *Marco Pettini*

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