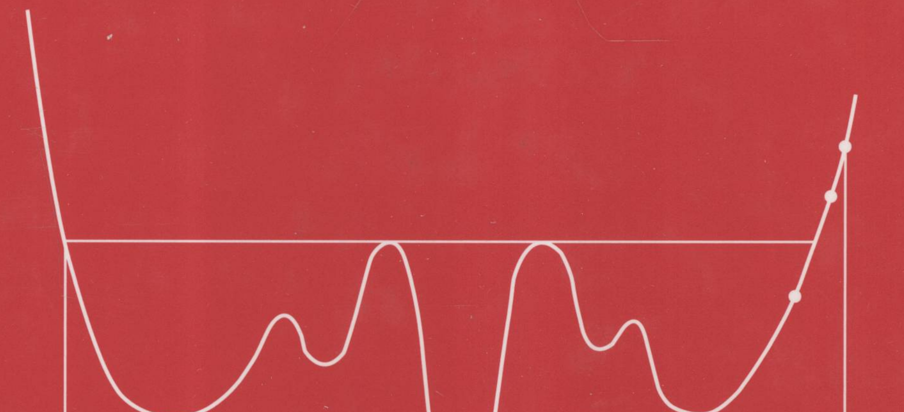
LARGE DEVIATIONS AND METASTABILITY

ENZO OLIVIERI AND MARIA EULÁLIA VARES



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CAMBRIDGE
UNIVERSITY PRESS

PUBLISHED BY THE PRESS SYNDICATE OF THE UNIVERSITY OF CAMBRIDGE
The Pitt Building, Trumpington Street, Cambridge, United Kingdom

CAMBRIDGE UNIVERSITY PRESS
The Edinburgh Building, Cambridge CB2 2RU, UK
40 West 20th Street, New York, NY 10011-4211, USA
477 Williamstown Road, Port Melbourne, VIC 3207, Australia
Ruiz de Alarcón 13, 28014 Madrid, Spain
Dock House, The Waterfront, Cape Town 8001, South Africa

http://www.cambridge.org

First published 2005

Printed in the United Kingdom at the University Press, Cambridge

Typeface Times 10/13 pt. *System* LaTeX 2_ε [TB]

A catalogue record for this book is available from the British Library

Library of Congress Cataloguing in Publication data

ISBN 0 521 59163 5 hardback

Large deviations and metastability

The book provides a general introduction to the theory of large deviations and a wide overview of the metastable behaviour of stochastic dynamics. With only minimal prerequisites, the book covers all the main results and brings the reader to the most recent developments. Particular emphasis is given to the fundamental Freidlin–Wentzell results on small random perturbations of dynamical systems. Metastability is first described on physical grounds, following which more rigorous approaches are developed. Many relevant examples are considered from the point of view of the so-called pathwise approach. The first part of the book develops the relevant tools, including the theory of large deviations, which are then used to provide a physically relevant dynamical description of metastability. Written to be accessible to graduate students, this book provides an excellent route into contemporary research.

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To Anna and Daniela, Juliana, Lucas and Vladas

PREFACE

This book has germinated from the lecture notes of a course 'Large deviations and metastability' given by one of us at the 'CIMPA First School on Dynamical and Disordered Systems', at Universidad de la Frontera, Temuco, during the summer of 1992 [293].

Since then a large amount of new material on metastability has been accumulated, and our goal was to combine a basic introduction to the theory of large deviations with a wide overview of the metastable behaviour of stochastic dynamics.

Typical examples of metastable states are supersaturated vapours and magnetic systems with magnetization opposite to the external field. Metastable behaviour is characterized by a long period of apparent equilibrium of a pure thermodynamic phase followed by an unexpected fast decay towards the stable equilibrium of a different pure phase or of a mixture, e.g. homogeneous nucleation of the liquid phase inside a highly supersaturated vapour, due to spontaneous density fluctuations. The point of view of metastability as a genuinely dynamical phenomenon is now widely accepted. Approaches which aim to describe static aspects of metastability (such as determination of the metastable branch of the equation of state of a fluid) in the Gibbs equilibrium set-up are, in their 'naïve form', applicable only in a mean field context. In this case, the physically unacceptable assumption that the range of the interaction equals the linear dimension of the container gives rise to pathological behaviour of non-convex free energy that implies negative compressibility, namely, thermodynamic instability. It is this feature that gives rise to the idea of associating metastability with local minima of the free energy. Moreover, dynamical aspects such as the lifetime of the metastable state require an investigation that a static approach is programmatically unable to provide. Thus, metastability for short range systems is included in the field of non-equilibrium statistical mechanics. Since a general theory of non-equilibrium thermodynamic phenomena is still lacking, a particularly relevant role is played by the study of specific mathematical models, for instance the stochastic Ising model.

The first attempt to formulate a rigorous dynamical theory of metastability goes back to Lebowitz and Penrose (see [240, 241]). In their approach the decay from metastability to stability is essentially characterized by a slow irreversible evolution of the expected values of the observables during the process. In [48] another method was proposed, based on a pathwise analysis of the process. The single trajectories of the process are characterized by a long period of random oscillations in apparent equilibrium (with a relatively fast loss of memory of the initial condition) followed by a sudden decay towards another, different regime, corresponding to stable equilibrium. In this approach metastability becomes strictly related to the first exit problem from special domains. Characterization of the most probable exit mechanism involves comparison between different rare events – a typical problem in large deviation theory.

After describing metastability on physical grounds, we present the existing rigorous approaches, with a particular emphasis on the pathwise approach, the main object of our analysis. Large deviation theory is applied, in combination with specific tools, to provide a dynamical description of metastability.

The construction of a mathematical theory of metastability not only provides interesting and physically relevant applications of the already established large deviation theory, but also poses new problems.

The first part of the book provides a reasonably self-contained account of basic results about large deviation theory. In Chapter 1 we discuss the classical basic results in the frame of large deviations for sums of independent random variables. In Chapter 2 we concentrate on the results of Freidlin and Wentzell in the context of small random perturbations of deterministic flows. Chapter 3 is mainly dedicated to the treatment of large deviations for interacting systems, and to its role in equilibrium statistical mechanics. The first two sections contain a short summary of large deviations for Markov chains and the Gärtner–Ellis theorem. The third section provides a brief introduction to equilibrium statistical mechanics, and the last section discusses large deviations for Gibbs measures and its relation to thermodynamical formalism.

In Chapter 4 we start the description of the metastability phenomenon and the various rigorous approaches to its treatment. The pathwise approach, which is one of the main topics of the book, is introduced in Section 4.2. The next two sections contain two examples: first we consider the extremely simple mean field model of the Curie–Weiss chain. Though unphysical, this mean field model can be considered as an initial 'laboratory', due to the explicitness of computations. The second example is the one-dimensional Harris contact process, which presents a non-trivial spatial structure. In the final section, we briefly outline results on metastability for other mean field type dynamics as well as the multidimensional Harris contact process. In Chapter 5 we are concerned with the verification of metastability for Itô processes in the context of the Freidlin–Wentzell theory. This is done in Section 5.4, based on results of Freidlin and Wentzell combined with coupling techniques. The important example of a double well potential is discussed in detail in Section 5.2. Finally, extensions to infinite dimensional situations such as reaction–diffusion models are briefly discussed at the end of the chapter.

In Chapter 6 we study the long time behaviour of general reversible Freidlin–Wentzell Markov chains; these are characterized by a finite state space and transition probabilities exponentially small in an external parameter that in many applications is the inverse temperature. In particular we analyse the first exit problem from particular sets of states, called *cycles*, whose characteristic property is that all their points are typically visited before the exit. Various aspects that are relevant for the description of metastable behaviour are studied: the asymptotic exponentiality of properly renormalized first exit times, the conditional equilibrium (Gibbs) measure, the 'tube' of typical trajectories during the exit.

In Chapter 7 we study metastability and nucleation for various short range lattice spin models that can be seen as generalizations of the standard stochastic Ising model. We consider the asymptotic regime with fixed volume and coupling constants in the limit of very low temperature. From a physical point of view this corresponds to the study of local aspects of nucleation; from a mathematical point of view it corresponds to the study of some large deviation phenomena for a class of Freidlin–Wentzell Markov chains. To study these models we apply the general results of Chapter 6 and have to solve some specific model dependent variational problems.

A particular emphasis is given to the case of reversible stochastic evolutions. Under the reversibility condition, many different dynamics such as quite general mean field models, Itô stochastic differential equations of gradient type, and stochastic Ising models can be treated by the same methods.

Parts of this text have been used in graduate courses at IMPA, Rio de Janeiro, and at Università di Roma 'Tor Vergata'. We would like to thank D. Tranah for the invitation to write this book, for his patience, attention and professionalism which made the process run smoothly during all these years.

The authors wish to thank all the colleagues who contributed in various ways to the realization of this work. Special thanks to A. Bovier, R. Cerf, F. den Hollander, S. Friedli, V. Gayrard, A. Gaudilliere, Ch. Gruber, H. Kesten, R. Kotecky, T. Mountford, O. Penrose and G. Sewell, for discussions on specific points or on general aspects of metastability. We are deeply grateful to E. Andjel, S. Brassesco, E. Cirillo, S. Carmona, A. Hinojosa, F. Manzo and F. Nardi, for reading parts of the text, making corrections, comments and suggestions which helped us to improve the presentation and correct several defects. We are particularly indebted to M. Cassandro, C.-E. Pfister, P. Picco, E. Presutti, R. Schonmann, E. Scoppola and V. Sidoravicius for their criticism, for many stimulating conversations, and for the clarifications they offered us through many discussions. Finally we would like to express gratitude to our families: Anna and Daniela, Juliana, Lucas and Vladas, for their patience and constant support, specially in the hardest moments of the long preparation of this book.

E. O. and M. E. V. acknowledge the warm hospitality of IMPA, Rio de Janeiro, and the Department of Mathematics at the Università di Roma 'Tor Vergata', respectively.

M. E. V. acknowledges financial support of CNPq and Faperj. This work has also received support from the CNPq-CNR scientific cooperation agreement.

Corrections that may appear in the future will be posted at
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Illud in his rebus non est mirabile, quare,
Omnia cum rerum primordia sint in motu,
Summa tamen summa videatur stare quiete,
Praeterquam siquid proprio dat corpore motus.

Lucretius, *De rerum natura*

CONTENTS

1

Large deviations: basic results

Introduction

In the analysis of a system with a large number of interacting components (at a microscopic level) it is of clear importance to find out about its collective, or macroscopic, behaviour. This is quite an old problem, going back to the origins of statistical mechanics, in the search for a mathematical characterization of 'equilibrium states' in thermodynamical systems. Though the problem is old, and the foundations of equilibrium statistical mechanics have been settled, the general question remains of interest, especially in the set-up of non-equilibrium systems. We could then take as the object of study a (non-stationary) time evolution with a large number (n) of components, where the initial condition and/or the dynamics present some randomness. One example of such a collective description is the so-called hydrodynamic limit. Passing by a space-time scale change (micro $\rightarrow$ macro) it allows, through a limiting procedure, the derivation of a reduced description in terms of macroscopic variables, such as density and temperature. Other limits, besides the hydrodynamic, may also appear in different situations, giving rise to macroscopic equations.

In all such cases the macroscopic equation indicates the *typical* behaviour in a *limiting situation* ($n \rightarrow +\infty$, and proper rescaling). Thus, it is essential to know something about:

(i) rates of convergence, i.e. how are the fluctuations of the macroscopic random fields (for example, the empirical density) around the prescribed value given by the macroscopic equation?

(ii) how to estimate the chance of observing something quite different than what is prescribed by the macroscopic equation. According to the prescription of the macroscopic equation these are 'rare events' and their probabilities will tend to zero, but *at which speed*?

In the above description we identify the three most basic limit theorems in classical probability: the macroscopic description corresponds to a 'law of large numbers'; the behaviour of the fluctuations, or 'moderate deviations', fits into the frame of a 'central limit theorem'; and the estimates of the probability of rare events constitute what are usually called 'large deviation principles'. The program for investigating the collective behaviour for evolutions given by Markov processes on $\{0, 1\}^{\mathbb{Z}^d}$ or $\mathbb{N}^{\mathbb{Z}^d}$, has grown since the 1980s (see [79]), and has taken definite forms for a class of them, cf. [78, 178, 283]. The situation is much less developed in the context of mechanical systems (see [283]).

The content of this book is closely related to questions such as (ii) above, and in particular to their connection with metastability, which will be discussed from Chapters 4 to 7. Perhaps we should say a few words on possible motivations for such estimates, bearing in mind the collective description of large systems. For example, if one wants to investigate the behaviour of the system at time scales longer than those for which the macroscopic equation is valid, then it is necessary to pay attention to such 'large fluctuations', since they will eventually occur. The ability to compare their probabilities becomes a crucial point in order to predict the long-term behaviour of the system. The classic example is a tunnelling event between two stable points of the macroscopic equation. Somehow, this comparison can be seen as a first step: one would believe that the large fluctuation should occur in the *least improbable* way. Nevertheless, carrying out this long time analysis may present (technical or serious) difficulties. One instance where this has been done quite completely is that in which the dynamics is, in some sense, already macroscopic; more precisely, it is obtained by the addition of a small external noise to a non-chaotic dynamical system. This is the object of Freidlin and Wentzell's theory [122], which will be studied in Chapters 2 and 5 of this book, also in connection with the phenomenon of metastability.

One should stress how closely related are the three mentioned problems: derivation of macroscopic equations/law of large numbers, fluctuations, and large deviations. Large deviation estimates yield stronger statements on the convergence of macroscopic density fields. On the other hand, a standard method for the derivation of large deviation estimates involves the validity of a large class of deterministic macroscopic limits (law of large numbers). A very important example of such a connection comes from equilibrium theory, through the possibility of applying large deviations to obtain the equivalence of ensembles, as pointed out in the fundamental articles of Ruelle [257], and Lanford [189], which have stimulated intense research. This goes far beyond the scope of this book, as for instance, the questions related to phase separation and surface large deviations. A brief discussion will appear in Chapter 3, with indications to recent research articles.

As a usual set-up for large deviations we could take a sequence of probability measures $(\mu_n)_{n\geq 1}$ on some metric space M, weakly converging to a Dirac point measure at some $m \in M$, in the sense that $\lim_{n\to+\infty} \int f d\mu_n = f(m)$ for all $f: M \to \mathbb{R}$ continuous and bounded. (In our previous discussion, μ_n should represent the law of an observable such as the empirical density, m representing a macrostate such as an equilibrium density.) The goal is to find the speed at which $\mu_n(A)$ tends to zero, when A is a fixed measurable set staying at positive distance from m. In particular, one wishes to detect whether a fast, exponential decay happens, in the sense that there exists $I(A) \in (0, +\infty]$ such that

$$\mu_n(A) \approx e^{-nI(A)}. \tag{1.1}$$

Throughout the text, $\approx$ denotes logarithmic equivalence, i.e. (1.1) means $n^{-1} \log \mu_n(A) \to -I(A)$ as $n \to \infty$. (*Notation.* $\log = \log_e$ everywhere in this text.)

Let us assume that (1.1) holds for a certain class of sets A; let A and B be two disjoint sets for which it holds. Since $\mu_n(A \cup B) = \mu_n(A) + \mu_n(B)$ it follows at once that $\mu_n(A \cup B) \approx e^{-n \min\{I(A), I(B)\}}$. This might suggest $I(A)$ of the form

$$I(A) = \inf_{x\in A} I(x), \tag{1.2}$$

for some point function I, which would then be called a 'rate function'. If so, we cannot expect (1.1) to hold for all measurable sets A; to see this, consider for example continuous measures, so that $\mu_n\{x\} = 0$ for all points $x \in M$. If (1.1) were true for such sets, this would force I to be identically $+\infty$, incompatible with (1.1) and (1.2) for $A = M$. This means that some restriction on the sets for which (1.1) holds is needed. This will be discussed in the next two sections, where a possible set-up will be presented.

It is natural to ask why one chooses the logarithmic equivalence $\approx$ instead of a sharper estimate like the usual equivalence ($a_n \sim b_n$ iff $a_n/b_n \to 1$). Significant advantages of the previous choice (allowing polynomial errors in (1.1)) include simplicity and a wide range of applicability. On the other hand, 'exact' results are essential in many applications though in this text we shall not pursue them.

Moreover, situations are expected to occur where $I(A)$ could vanish, meaning that the decay is less than exponential, and that (1.1) does not provide enough information. In such cases, one definitely needs a more precise asymptotics.

For a comparison with 'moderate deviations' (central limit theorems), let us take $M = \mathbb{R}^d$. According to the previous notation, these refer to the asymptotics of $\mu_n(A_n)$ where $A_n = m + \alpha_n A$, $\alpha_n \to 0$ suitably, and A is fixed.

1.1 Cramér–Chernoff theorem on $\mathbb{R}$

Let us start with the simplest situation: the microstates correspond to the results of n independent tosses of a fair coin, and μ_n represents the law of the