Hans-Otto Georgii

Gibbs Measures and Phase Transitions

Second Edition

吉布斯测度和相变 第2版

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To my family

Preface

This book deals with systems of infinitely many random variables attached to the vertices of a multi-dimensional lattice and depending on each other according to their positions. The theory of such "spatial random systems with interaction" is a rapidly growing branch of probability theory developed with the goal of understanding the cooperative effects in large random systems. The primary impetus comes from statistical physics. The range of applications also includes various other fields such as biology, medicine, chemistry, and economics, but this volume is only devoted to those concepts and results which are significant for physics. In the physicist's terminology, this subject is referred to as classical (i.e. non-quantum) equilibrium statistical mechanics of infinite lattice systems.

As is well-known, statistical physics attempts to explain the macroscopic behaviour of matter on the basis of its microscopic structure. This effort also includes the analysis of simplified mathematical models. Consider, for example, the phenomenon of ferromagnetism. In a first approximation, a ferromagnetic metal (like iron) can be regarded as being composed of elementary magnetic moments, called spins, which are arranged on the vertices of a crystal lattice. The orientations of the spins are random but certainly not independent – they are subject to a spin-spin interaction which favours their alignment. It is plausible that this microscopic interaction is responsible for the macroscopic effect of spontaneous magnetization. What, though, are the essential features of the interaction giving rise to this phase transition? This sort of question is one of the motivations for the development and analysis of the stochastic models considered herein.

Although the foundations of statistical mechanics were already laid in the nineteenth century, the study of infinite systems only began in the late 1960s with the work of R.L. Dobrushin, O.E. Lanford, and D. Ruelle who introduced the basic concept of a Gibbs measure. This concept combines two elements, namely (i) the well-known Maxwell-Boltzmann-Gibbs formula for the equilibrium distribution of a physical system with a given energy function, and (ii) the familiar probabilistic idea of specifying the interdependence structure of a family of random variables by means of a suitable class of conditional probabilities. One of the interesting features of this concept is the fact that (as a consequence of the implicit nature of the interdependence structure) a Gibbs measure for a given type of interaction may fail to be unique. In physical terms, this means that a physical system with this interaction can take several distinct equilibria. The phenomenon of non-uniqueness of a Gibbs measure

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can thus be interpreted as a phase transition and is, as such, of particular physical significance. The main topics of this book are, therefore, the problem of non-uniqueness of Gibbs measures, the converse problem of uniqueness, and the question as to the structure of the set of all Gibbs measures.

Due to its interdisciplinary nature, the theory of Gibbs measures can be viewed from different perspectives. The treatment here follows a probabilitistic, rather than a physical, approach. A prior knowledge of statistical mechanics is not required. The prerequisites for reading this book are a basic knowledge of measure theory at the level of a one-semester graduate course and, in particular, some familiarity with conditional expectations and probability kernels. The books by Bauer (1981) and Cohn (1980) contain much more than is needed. Some other tools which are used on occasion are a few standard results from probability theory and functional analysis such as the backward martingale convergence theorem and the separating hyperplane theorem. In all such cases a reference is given to help the uninitiated reader. My intention is that this monograph serve as an introductory text for a general mathematical audience including advanced graduate students, as a source of rigorous results for physicists, and as a reference work for the experts. It is my particular hope that this book might help to popularize its subject among probabilists, and thereby stimulate future research.

There are four parts to the book. Part I (the largest part) contains the elements of the theory: basic concepts, conditions for the existence of Gibbs measures, the decomposition into extreme Gibbs measures, general uniqueness results, a few typical examples of phase transition, and a general discussion of symmetries. The other parts are largely independent of one another. Part II contains a collection of results closely related to some classical chapters of probability theory. The central objects of study are Markov fields and Markov chains on the integers and on trees, as well as Gaussian fields on $\mathbb{Z}^d$ and other lattices. Part III is devoted to spatially homogeneous Gibbs measures on $\mathbb{Z}^d$. The topics include the ergodic decomposition, a variational characterization of shift-invariant Gibbs measures, the existence of phase transitions of prescribed types and a density theorem for ergodic Gibbs measures. Part IV deals with the existence of phase transitions in shift-invariant models on $\mathbb{Z}^d$ which satisfy a definiteness condition called reflection positivity. The non-uniqueness theorems provided here can be applied to various kinds of specific models having one of the following characteristic features: a stable degeneracy of ground states, a competition of several potential wells of different depths, or the existence of an $SO(N)$-symmetry.

Each part and each chapter begins with an introductory paragraph which may be consulted for further information on the contents and the interdependence of chapters. The Introduction is primarily addressed to readers who are not familiar with statistical physics. It provides some motivation for the definition of a Gibbs measure and indicates why the phenomenon of non-uniqueness can be interpreted as a phase transition. Many of the general notations of this book are already introduced in Section 1.1, but some standard mathematical notations are only explained in the List of Symbols at the end. With only a few exceptions, all historical and bibliographical comments are collected in a separate section, the "Bibliographical Notes". This section also includes a brief outline of numerous results which are not treated in the text, but this is by no means a full account of the vast literature. The bibliography contains only those papers which are referred to in the Bibliographical Notes or somewhere else in the book.

A few words about the limitations of scope are appropriate. As stated above, this book is devoted to lattice models of classical statistical physics. It therefore neither contains a treatment of quantum-machanical models nor an analysis of interacting point particles in Euclidean space. Moreover, this book does not include a discussion of lattice systems with random interaction such as diluted ferromagnets and spin glass models, although this is a field of particular current interest. Even with these restrictions, the subject matter exceeds by far that which can be presented in detail in a single volume. There are two major omissions in this book: the Pirogov-Sinai theory of low-temperature phase diagrams, and the immense field of ferromagnetic correlation inequalities and their applications. A sketch of these subjects can be found in the Bibliographical Notes (especially those on Chapters 2 and 19), and I urge the reader to investigate the literature given there. Also, since readability rather than generality has been my goal, systems of genuinely unbounded spins are treated here only sporadically rather than systematically, although references are given in the Bibliographical Notes. Some further topics which are not even touched upon are the field of "exactly solved" lattice models such as the eight- and six-vertex models (cf. Baxter (1982a)), the significance of unbounded spin systems for constructive quantum field theory (cf. Simon (1974), Guerra et al. (1975), and Glimm and Jaffe (1981)), lattice gauge theories (cf. Seiler (1982)), and stochastic time evolutions having Gibbs measures for their stationary measures (cf. Durrett (1981) and Liggett (1985) as well as Doss and Royer (1978) and Holley and Stroock (1981), e.g.).

Finally, I take this opportunity to thank my academic teacher Konrad Jacobs for advice and encouragement during my first years as a probabilist, and in particular for guiding my interest towards the probabilistic problems of statistical mechanics. For many years, I had the good fortune of working in the groups of Hermann Rost in Heidelberg and Chris Preston in Bielefeld, and I gratefully acknowledge their influence on my work. I am particularly indebted to Paul Deuring, Aernout van Enter, József Fritz, Andreas Greven, Harry Kesten, Hans-Rudolf Künsch, Reinhard Lang, Fredos Papangelou, Michael Röckner, and Herbert Spohn for reading various portions of the manuscript and making numerous valuable comments. Pól Mac Aonghusa looked over the English, and Mrs. Christine Hele typed the manuscript with

care and patience. Last but not least, I would like to express my gratitude to the editors of this series, in particular Heinz Bauer, for their stimulating interest in this project.

Munich, May 1988 *Hans-Otto Georgii*

Preface to the Second Edition

A second edition after 23 years of rapid development of the field? One may well say that this should give reason for a complete rewriting of the book. But, on the other hand, a selection of topics had to be made already in the first edition, and this particular selection has found its firm place in the literature. In view of this and some technical restrictions, the publisher and I decided to keep the book more or less in its previous state and to make only modest changes. Apart from the correction of a few minor errors which were already fixed in the Russian edition (Moscow: Mir 1992) and some small adjustments, these changes are

- a new section, 15.5, on large deviations for Gibbs measures and the minimum free energy principle, and
- a brief overview of the main progress since 1988, which is added to the Bibliographical Notes.

In particular, the latter will show that many of the omissions here are filled by other texts. My thanks go to Anton Bovier, Franz Merkl, Herbert Spohn and especially Aernout van Enter for valuable comments on a first draft of the second addendum. I am also grateful to the publisher and the series editors for their constant interest in this work.

Munich, January 2011 *Hans-Otto Georgii*

Contents

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Introduction

The theory of Gibbs measures is a branch of Classical Statistical Physics but can also be viewed as a part of Probability Theory. The notion of a Gibbs measure dates back to R.L. Dobrushin (1968–1970) and O.E. Lanford and D. Ruelle (1969) who proposed it as a natural mathematical description of an equilibrium state of a physical system which consists of a very large number of interacting components. In probabilistic terms, a Gibbs measure is nothing other than the distribution of a countably infinite family of random variables which admit some prescribed conditional probabilities. During the two decades since 1968, this notion has received considerable interest from both mathematical physicists and probabilists. The physical significance of Gibbs measures is now generally accepted, and it became evident that the physical questions involved give rise to a variety of fascinating probabilistic problems. In this introduction we shall give an outline of some physical grounds which motivate the definition of, and justify the interest in, Gibbs measures.

The physical background. Consider, for example, a piece of a ferromagnetic metal (like iron, cobalt, or nickel) in thermal equilibrium. The piece consists of a very large number of atoms which are located at the sites of a crystal lattice. Each atom shows a magnetic moment which can be visualized as a vector in $\mathbb{R}^3$. Since this magnetic moment results from the angular moments, the so-called spins, of the electrons, it is also called, for short, the spin of the atom. The interaction properties of the electrons in the crystal imply that any two adjacent atoms have a tendency to align their spins in parallel. At high temperatures, this tendency is compensated by the thermal motion. If, however, the temperature is below a certain threshold value which is called the Curie temperature, the coupling of moments dominates and gives rise to the phenomenon of spontaneous magnetization: Even in the absence of any external field, the atomic spins align and thus induce a macroscopic magnetic field. In a variable external field h, the magnetization of the ferromagnet thus exhibits a jump discontinuity at $h = 0$. (As a matter of fact, a real ferromagnet falls into several so-called Weiss domains with different directions of magnetization. We ignore this effect which is superimposed on the above behaviour. In other words, we are only interested in the intrinsic properties of a single Weiss domain.)

As a second example from Statistical Physics we consider the liquid-vapour phase transition of a real gas. On the macroscopic level, this phase transition is again characterized by a jump discontinuity, namely a jump of the density of the gas as a function of the pressure (at a fixed value of temperature). This analogy between real gases and ferromagnets also extends to the microscopic level, at least if we adopt the following simplified picture of a gas. The gas consists of a huge number of particles which interact via van der Waals forces. To describe the spatial distribution of the particles we may imagine that the container of the gas is divided into a large number of cells which are of the same order of magnitude as the particles. To each cell we assign its occupation number, i.e. the number of particles in the cell. (More generally, we could also distinguish between particles of different types and/or orientations.) We also replace the van der Waals attraction between the particles by an effective interaction between the occupation numbers. The resulting caricature of a gas is called a *lattice gas*. In spite of all defects of this reduced picture, one might expect that a lattice gas still exhibits a liquid-vapour phase transition. From a formal point of view, this transition is similar to the spontaneous magnetization of a ferromagnet: The cells in the container correspond to the ferromagnetic atoms, and the occupation numbers correspond to the magnetic moments.

The mathematical model. How can a ferromagnet or a lattice gas in thermal equilibrium be described in mathematical terms? As we will show now, this question leads to the concept of a Gibbs measure. We shall proceed in four steps.

Step 1: The configuration space. What are the common features of a ferromagnet and a lattice gas? First, there is a large (but finite) set S which labels the components of the system. In the case of a ferromagnet, S consists of the sites of the crystal lattice which is formed by the positions of the atoms. In a lattice gas, S is the set of all cells which subdivide the volume which is filled with the gas. Secondly, there is a set E which describes the possible states of each component. For a ferromagnet, E is the set of all possible orientations of the magnetic moments. For example, to design a simple model we might assume that each moment is only capable of two orientations. Then $E = \{-1, 1\}$, where 1 stands for "spin up" and -1 for "spin down". In the case of a lattice gas, we can take $E = \{0, 1, \dots, N\}$, where N is the maximal number of particles in a cell. In the simplest case we have $E = \{0, 1\}$, where 1 stands for "cell is occupied" and 0 for "cell is empty". Having specified the sets S and E, we can describe a particular state of the total system by a suitable element $\omega = (\omega_i)_{i \in S}$ of the product space $\Omega = E^S$. Ω is called the configuration space.

Step 2: The probabilistic point of view. The physical systems considered above are characterized by a sharp contrast: The microscopic structure is enormously complex, and any measurement of microscopic quantities is subject to statistical fluctuations. The macroscopic behaviour, however, can be described by means of a few parameters such as temperature and pressure resp. magnetization, and macroscopic measurements lead to apparently deterministic results. This contrast between the microscopic and the macroscopic level is the starting point of Classical Statistical Mechanics as developed by Maxwell, Boltzmann, and Gibbs. Their basic idea may be summarized as follows: The microscopic complexity can be overcome by a statistical approach; the macroscopic determinism then may be regarded as a consequence of a suitable law of large numbers. According to this philosophy, it is not adequate to describe the state of the system by a particular element ω of the configuration space Ω. The system's state should rather be described by a family $(\sigma_i)_{i \in S}$ of E-valued random variables, or (if we pass to the joint distribution of these random variables) by a probability measure μ on Ω. Of course, the probability measure μ should be consistent with the available partial knowledge of the system. In particular, μ should take account of the a priori assumption that the system is in thermal equilibrium.

Step 3: The Gibbs distribution. Which kind of probability measure on Ω is suitable to describe a physical system in equilibrium? The term "equilibrium" clearly refers to the forces that act on the system. Thus, before specifying a probabilistic model of an equilibrium state we need to specify a Hamiltonian H which assigns to each configuration ω a potential energy $H(\omega)$. In the physical systems above, the essential contribution to the potential energy comes from the interaction of the microscopic components of the system. In addition, there may be an external force.

For example, in the case of a ferromagnet with state space $E = \{-1, 1\}$ it is reasonable to consider a Hamiltonian of the form

$$(0.1) \qquad H(\omega) = - \sum_{\{i,j\} \subset S} J(i,j)\omega_i\omega_j - h \sum_{i \in S} \omega_i.$$

Here $J(i,j) = J(j,i) > 0$, and h is real number. The term $-J(i,j)\omega_i\omega_j$ represents the interaction energy of the spins ω_i and ω_j. This energy is minimal if $\omega_i = \omega_j$, i.e. if ω_i and ω_j are aligned, the interaction is thus ferromagnetic. The number h represents the action of an external magnetic field. (If $h > 0$, this field is oriented in the positive direction of the spins.) A Hamiltonian of the form (0.1) can also be used in the case of a lattice gas with state space $E = \{0, 1\}$. In this case, the term $-J(i,j)\omega_i\omega_j$ is only non-zero when the cells i and j are occupied; hence $-J(i,j)$ is the interaction energy of the two particles in these cells, and the condition $J(i,j) > 0$ means that the particles attract each other. In the lattice gas context, h is to be interpreted as a chemical potential, i.e., h represents the work which is necessary in order to place a particle in the system.

As soon as we have specified a Hamiltonian H, the answer to the question which was posed at the beginning of this step is provided by Statistical Mechanics: The equilibrium state of a physical system with Hamiltonian H is described by the probability measure

$$(0.2) \qquad \mu(d\omega) = Z^{-1} \exp[-\beta H(\omega)]\, d\omega$$

on Ω. In this expression, the notation $d\omega$ refers to a suitable a priori measure on Ω (for example, the counting measure if Ω is finite), β is a positive number which is proportional to the inverse of the absolute temperature, and $Z > 0$ is a normalizing constant. The above μ is called the *Gibbs distribution* (or, somewhat old-fashioned, the *Gibbs ensemble*) relative to H. (In the ferromagnetic context, μ is the so-called canonical Gibbs distribution. In the lattice gas case, μ is the grand canonical distribution). The rigorous justification of the ansatz (0.2) is a long story which is still far from being finished. We just mention the key words "ergodic hypothesis", "equivalence of ensembles", and "second law of thermodynamics". In the meantime, the prescription (0.2) may be regarded as a postulate which is justified by its stupendous success.

Step 4: The infinite volume limit. As we have emphasized above, the number of atoms in a ferromagnet and the number of microscopic cells in a lattice gas are extremely large. Consequently, the set S in our mathematical model should be very large. According to a standard rule of mathematical thinking, the intrinsic properties of large objects can be made manifest by performing suitable limiting procedures. It is therefore a common practice in Statistical Physics to pass to the infinite volume limit $|S| \to \infty$. (This limit is also referred to as the thermodynamic limit.) However, instead of performing the same kind of limit over and over it is often preferable to study directly the class of all possible limiting objects. In our context, this means that the finite lattice S should be replaced by a countably infinite lattice such as, for example, the d-dimensional integer lattice $\mathbb{Z}^d$. We are thus led to a study of systems with infinitely many interacting components, and we are faced with the problem of describing an equilibrium state of such a system by a suitable probability measure on an infinite product space like $\Omega = E^{\mathbb{Z}^d}$. However, if S is an infinite lattice and the interaction is spatially homogeneous then a Hamiltonian like (0.1) is no longer well-defined, and formula (0.2) thus makes no sense. To overcome this obstacle we either might consider limits of suitable Gibbs distributions as S increases to an infinite lattice; this, however, turns out to be rather difficult in general. Alternatively, we might try to characterize the Gibbs distribution (0.2) by a property which admits a direct extension to the case of an infinite lattice. Such a characterization can indeed be obtained fairly easily, as we will now show. (In fact, this characterization will lead us to a result which is intimately connected with what can be obtained by suitable limits; cf. (4.17) and (7.30) in the text).

To be specific we let $E = \{-1, 1\}$ or $\{0, 1\}$, S be finite, and H be given by (0.1). We also let Λ be any non-empty subset of S and $\zeta \in E^\Lambda$ and $\eta \in E^{S\setminus\Lambda}$ any two configurations on Λ resp. the complement $S\setminus\Lambda$; the combined configuration on S will be denoted $\zeta\eta$. We consider the probability of the event "ζ occurs in Λ" under the hypothesis "η occurs in $S\setminus\Lambda$" relative to the probability measure μ in (0.2). ($d\omega$ is counting measure.) Cancelling all terms which only depend on η, we find that

$$(0.3)\qquad \mu(\zeta \text{ in } \Lambda | \eta \text{ in } S\setminus\Lambda) = \mu(\zeta\eta \text{ in } S)/\mu(\eta \text{ in } S\setminus\Lambda) = \exp[-\beta H(\zeta\eta)] \Big/ \sum_{\tilde\zeta \in E^\Lambda} \exp[-\beta H(\tilde\zeta\eta)] = Z_\Lambda(\eta)^{-1} \exp[-\beta H_\Lambda(\zeta\eta)].$$

Here

$$H_\Lambda(\zeta\eta) = -\sum_{\{i,j\}\subset\Lambda} J(i,j)\zeta_i\zeta_j - \sum_{i\in\Lambda} \zeta_i \left[h + \sum_{j \in S\setminus\Lambda} J(i,j)\eta_j \right],$$

considered as a function of ζ, is the Hamiltonian of the subsystem in Λ with "boundary condition" η, and

$$Z_\Lambda(\eta) = \sum_{\tilde\zeta \in E^\Lambda} \exp[-\beta H_\Lambda(\tilde\zeta\eta)]$$

is a normalizing constant. Conversely, there is only one μ which satisfies (0.3) for all ζ, η, and Λ, namely the Gibbs distribution (0.2). (To see this it is sufficient to put $\Lambda = S$.) Since each $\Lambda \subset S$ is automatically finite, we can conclude that the probability measure μ in (0.2) is uniquely determined by the property that each finite subsystem, conditioned on its surroundings, has a Gibbsian distribution relative to the Hamiltonian that belongs to this subsystem. Now the point is that the last property still makes sense when the lattice S is infinite. We are thus led to the following definition of an infinite-lattice counterpart of a Gibbs distribution:

Consider a probability measure μ on a product space $\Omega = E^S$, where S is countably infinite and E is any measurable space. μ is called a *Gibbs measure* if, for each *finite* subset Λ of S and μ-almost every configuration η outside Λ, the conditional distribution of the configuration in Λ given η is Gibbsian relative to the Hamiltonian in Λ with boundary condition η. The family $\gamma = (\gamma_\Lambda(\cdot|\eta))_{\eta,\Lambda}$ of all these Gibbsian conditional distributions is called the *specification* of μ. γ describes the interdependencies between the configurations on different parts of S; these interdependencies are dictated by the interaction between the components of the system.

Let us summarize the above paragraphs as follows: *A Gibbs measure is a mathematical idealization of an equilibrium state of a physical system which consists of a very large number of interacting components.* In the language of Probability Theory, *a Gibbs measure is simply the distribution of a stochastic process which, instead of being indexed by the time, is parametrized by the sites of a spatial lattice, and has the special feature of admitting prescribed versions of the conditional distributions with respect to the configurations outside finite regions.*

As is evident from the last sentence, there is a formal analogy between Gibbs measures and Markov processes. This analogy contributes to the purely probabilistic interest in Gibbs measures. (As a matter of fact, there are some

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