Lecture Notes in Mathematics

1970

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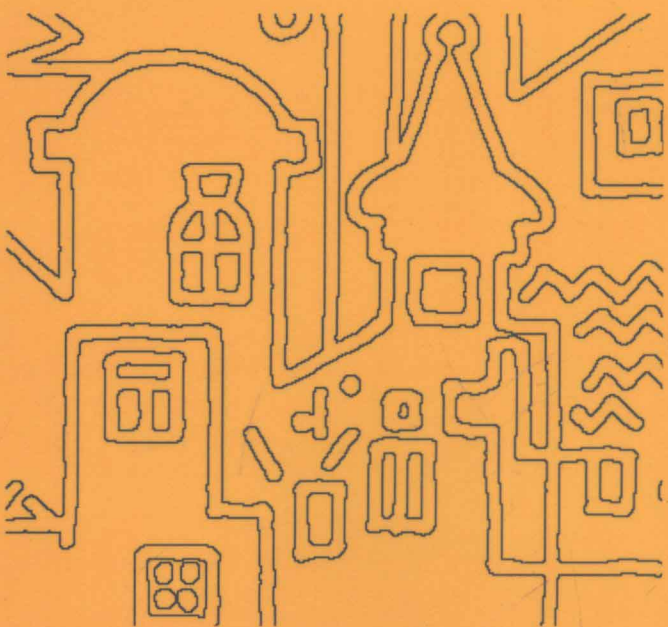
Methods of Contemporary Mathematical Statistical Physics

Editor: Roman Kotecký



Springer

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ISBN: 978-3-540-92795-2 e-ISBN: 978-3-540-92796-9
DOI: 10.1007/978-3-540-92796-9

Lecture Notes in Mathematics ISSN print edition: 0075-8434
ISSN electronic edition: 1617-9692

Library of Congress Control Number: 2009920693

Mathematics Subject Classification (2000): 82B20, 82B26, 82C20, 60K35, 82C26, 82C35, 82B31, 82B41, 82B44, 82B10, 82C22, 60K05, 82B05, 82C05

Cover picture by Pavel Brázda

Cover design: SPi Publisher Services

Printed on acid-free paper

springer.com

Preface

The Lecture Notes collect seven mini-courses presented at the 5th Prague Summer School on Mathematical Statistical Physics that took place during two weeks of September 2006. As with preceding schools, it was aimed at PhD students and young postdocs. The central theme of the volume is what could be called "mathematics of phase transitions" in diverse contexts. Even though all courses were meant to introduce the reader to recent progress of a particular topic of modern statistical physics, attention has been paid to providing a solid grounding by carefully developing various basic tools.

One of the techniques that led, more than two decades ago, to a series of important outcomes in the theory of phase transitions of lattice models was reflection positivity. Recently it resurfaced and was used to obtain interesting new results in various settings. The lectures of Marek Biskup include a thorough introduction to reflection positivity as well as a review of its recent applications. In addition, it contains a crash course on lattice spin models that is useful as a background for other lectures of the collection.

Also the following two contributions concern equilibrium statistical physics. The lectures of Dmitri Ioffe are devoted to a stochastic geometric reformulation of classical as well as quantum Ising models. A unified approach to the Fortuin-Kasteleyn and random current representations in terms of path integrals is presented.

Statistical mechanics of directed polymers interacting with one-dimensional spatial effects is a topic with various applications in physics and biophysics. The lectures of Fabio Toninelli are devoted to a thorough discussion of the localization/delocalization transition in these models.

Metastability is a topic that has attracted a lot of attention recently. Here it is discussed in the notes of Anton Bovier and Frank den Hollander. The emphasis of the course of Anton Bovier is on a general rigorous framework. It explores how distinct time scales arise in Markov processes and how the metastable exit times can be expressed in terms of capacity, the crucial notion coming from potential theory. The lectures by Frank den Hollander are then devoted to a nontrivial application to metastability in the context of Glauber and Kawasaki dynamics of lattice gases. The main step is the careful evaluation of the relevant capacity in these particular cases.

Readers can have a glimpse of the prolifically developing nonequilibrium realm in the remaining two contributions. The lectures that were presented by Christian Maes and Karel Netočný form a pedagogical account of several recently discussed topics, with an emphasis on general principles.

Facilitated spin models, also known as kinetically constrained spin models, are reflecting important peculiar features of glassy dynamics. The lectures of Fabio Martinelli, submitted here with his coauthors, review mathematical results that contributed to a settlement of questions arising from numerical simulations.

Only one mini-course presented in Prague was not included into the present volume. These are the lectures about computational complexity and phase transitions in combinatorial optimisation presented by Stefan Mertens. The main reason for this ommision is that his presentation was based on the recent monograph written by him and Cris Moore that already covers very well this topic.

The School was organised by Center for Theoretical Study (through the grant MSM 0021620845) with the Institute of Theoretical Computer Science at Charles University providing their beautiful lecture room in the historical centre. It could not have happened without the support of the European Science Foundation under the auspices of the programme Phase Transitions and Fluctuation Phenomena for Random Dynamics in Spatially Extended Systems. But most of all, the success of the School was determined by the lecturers as well as the students who created a pleasant and stimulating atmosphere. We hope that this spirit found its way into the written version of the lecture notes and will be appreciated by the reader.

Prague
November, 2008

Roman Kotecký

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Reflection Positivity and Phase Transitions in Lattice Spin Models

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R. Kotecký (ed.), *Methods of Contemporary Mathematical Statistical Physics*, Lecture Notes in Mathematics 1970, DOI: 10.1007/978-3-540-92796-9_1,

1 Introduction

Phase transitions are one of the most fascinating, and also most perplexing, phenomena in equilibrium statistical mechanics. On the physics side, many approximate methods to explain or otherwise justify phase transitions are known but a complete mathematical understanding is available only in a handful of simplest of all cases. One set of tractable systems consists of the so called *lattice spin models*. Originally, these came to existence as simplified versions of (somewhat more realistic) models of crystalline materials in solid state physics but their versatile nature earned them a life of their own in many other disciplines where complex systems are of interest.

The present set of notes describes one successful *mathematical* approach to phase transitions in lattice spin models which is based on the technique of *reflection positivity*. This technique was developed in the late 1970s in the groundbreaking works of F. Dyson, J. Fröhlich, R. Israel, E. Lieb, B. Simon and T. Spencer who used it to establish phase transitions in a host of physically-interesting classical and quantum lattice spin models; most notably, the classical Heisenberg ferromagnet and the quantum XY model and Heisenberg antiferromagnet. Other powerful techniques — e.g., Pirogov-Sinai theory, lace expansion or multiscale analysis in field theory — are available at present that can serve a similar purpose in related contexts, but we will leave their review to experts in those areas.

The most attractive feature of reflection positivity — especially, compared to the alternative techniques — is the simplicity of the resulting proofs. There are generally two types of arguments one can

use: The first one is to derive the so called *infrared bound*, which states in quantitative terms that the fluctuations of the spin variables are dominated by those of a lattice Gaussian free field. In systems with an internal symmetry, this yields a proof of a symmetry-breaking phase transition by way of a spin-condensation argument. Another route goes via the so called *chessboard estimates*, which allow one to implement a Peierls-type argument regardless of whether the model exhibits an internal symmetry or not.

Avid users of the alternative techniques are often quick to point out that the simplicity of proofs has its price: As a rather restrictive condition, reflection positivity applies only to a small (in a well defined sense) class of systems. Fortunately for the technique and mathematical physics in general, the models to which it does apply constitute a large portion of what is interesting for physics, *and* to physicists. Thus, unless one is exclusively after universal statements — i.e., those robust under rather arbitrary perturbations — the route via reflection positivity is often fairly satisfactory.

The spectacular success of reflection positivity from the late 1970s was followed by many interesting developments. For instance, in various joint collaborations, R. Dobrushin, R. Kotecký and S. Shlosman showed how chessboard estimates can be used to prove a phase transition in a class of systems with naturally-defined ordered and disordered components; most prominently, the q-state Potts model for $q \gg 1$. Another neat application came in the papers of M. Aizenman from early 1980s in which he combined the infrared bound with his random-current representation to conclude mean-field critical behavior in the nearest-neighbor Ising ferromagnet above 4 dimensions. Yet another example is the proof, by L. Chayes, R. Kotecký and S. Shlosman, that the Fisher-renormalization scheme in annealed-diluted systems may be substituted by the emergence of an intermediate phase.

These notes discuss also more recent results where their author had a chance to contribute to the field. The common ground for some of these is the use of reflection positivity to provide mathematical justification of "well-known" conclusions from physics folklore. For instance, in papers by N. Crawford, L. Chayes and the present author, the infrared bound was shown to imply that, once a model undergoes a field or energy driven first-order transition in mean-field theory, a similar transition will occur in the lattice model provided the spatial dimension is sufficiently high or the interaction is sufficiently spread-out (but still reflection positive). Another result — due to L. Chayes, S. Starr and the present author — asserts that if a reflection-positive quantum

spin system undergoes a phase transition at intermediate temperatures in its classical limit, a similar transition occurs in the quantum system provided the magnitude of the quantum spin is sufficiently large.

There have also been recent cases where reflection positivity brought a definite end to a controversy that physics arguments were not able to resolve. One instance concerned certain non-linear vector and liquid-crystal models; it was debated whether a transition can occur already in 2 dimensions. This was settled in recent work of A. van Enter and S. Shlosman. Another instance involved spin systems whose (infinite) set of ground states had a much larger set of symmetries than the Hamiltonian of the model; two competing physics reasonings argued for, and against, the survival of these states at low temperatures. Here, in papers of L. Chayes, S. Kivelson, Z. Nussinov and the present author, spin-wave free energy calculations were combined with chessboard estimates to construct a rigorous proof of phase coexistence of only a *finite* number of low-temperature states.

These recent activities show that the full potential of reflection positivity may not yet have been fully exhausted and that the technique will continue to play an important role in mathematical statistical mechanics. It is hoped that the present text will help newcomers to this field learn the essentials of the subject before the need arises to plow through the research papers where the original derivations first appeared.

Organization

This text began as class notes for nine hours of lectures on reflection positivity at the 2006 Prague School and gradually grew into a survey of (part of) this research area. The presentation opens with a review of basic facts about lattice spin models and then proceeds to study two applications of the infrared bound: a spin-condensation argument and a link to mean-field theory. These are followed by the classical derivation of the infrared bound from reflection positivity. The remainder of the notes is spent on applications of a by-product of this derivation, the chessboard estimate, to proofs of phase coexistence.

The emphasis of the notes is on a *pedagogical* introduction to reflection positivity; for this reason we often sacrifice on generality and rather demonstrate the main ideas on the simplest case of interest. To compensate for the inevitable loss of generality, each chapter is endowed with a section "Literature remarks" where we attempt to list the references deemed most relevant to the topic at hand. The notes are closed with a short section on topics that are not covered as well as some open problems that the author finds worthy of some thought.

Acknowledgments

A review naturally draws on the work of many authors. We will do our best to give proper credit to their contribution in the sections "Literature remarks" that appear at the end of each chapter and, of course, in the list of references. I have personally learned a great deal of the subject from Lincoln Chayes with whom I have subsequently coauthored more than half-a-dozen papers some of which will be discussed here. During this time I also benefited from collaborations with N. Crawford, S. Kivelson, R. Kotecký, Z. Nussinov and S. Starr, and from various enlightening discussions involving A. van Enter, B. Nachtergaele and S. Shlosman.

The text would presumably never exist were it not for Roman Kotecký's summer school; I wish to thank him for allowing me to speak on this subject. I am indebted to the participants of the school for comments during the lectures and to T. Bodineau, A. van Enter, E. Lieb and S. Shlosman for suggestions on the first draft of the notes. My presence at the school was made possible thanks to the support from the ESF-program "Phase Transitions and Fluctuation Phenomena for Random Dynamics in Spatially Extended Systems" and from the National Science Foundation under the grant DMS-0505356.

2 Lattice Spin Models: Crash Course

This section prepares the ground for the rest of the course by introducing the main concepts from the theory of Gibbs measures for lattice spin models. The results introduced here are selected entirely for the purpose of these notes; readers wishing a more comprehensive — and in-depth — treatment should consult classic textbooks on the subject.

2.1 Basic Setup

Let us start discussing the setup of the models to which we will direct our attention throughout this course. The basic ingredients are as follows:

- *Lattice*: We will take the d-dimensional hypercubic lattice $\mathbb{Z}^d$ as our underlying graph. This is the graph with vertices at all points in $\mathbb{R}^d$ with integer coordinates and edges between any *nearest neighbor* pair of vertices; i.e., those at Euclidean distance one. We will use $\langle x, y \rangle$ to denote an (unordered) nearest-neighbor pair.

- *Spins*: At each $x \in \mathbb{Z}^d$ we will consider a spin S_x, by which we will mean a random variable taking values in a closed subset Ω of $\mathbb{R}^\nu$, for some $\nu \geq 1$. We will use $S_x \cdot S_y$ to denote a scalar product between S_x and S_y (Euclidean or otherwise).
- *Spin configurations*: For $\Lambda \subset \mathbb{Z}^d$, we will refer to $S_\Lambda := (S_x)_{x\in\Lambda}$ as the spin configuration in Λ. We will be generically interested in describing the statistical properties of such spin configurations with respect to certain (canonical) measures.
- *Boundary conditions*: To describe the law of S_Λ, we will not be able to ignore that some spins are also outside Λ. We will refer to the configuration S_{Λ^c} of these spins as the boundary condition. The latter will usually be fixed and may often even be considered a parameter of the game. When both S_Λ and S_{Λ^c} are known, we will write
$$S := (S_\Lambda, S_{\Lambda^c}) \tag{2.1}$$
to denote their concatenation on all of $\mathbb{Z}^d$.

The above setting incorporates rather varied physical contexts. The spins may be thought of as describing magnetic moments of atoms in a crystal, displacement of atoms from their equilibrium positions or even orientation of grains in nearly-crystalline granular materials.

To define the dynamics of spin systems, we will need to specify the energetics. This is conveniently done by prescribing the *Hamiltonian* which is a function on the spin-configuration space $\Omega^{\mathbb{Z}^d}$ that tells us how much energy each spin configuration has. Of course, to have all quantities well defined we need to fix a *finite* volume $\Lambda \subset \mathbb{Z}^d$ and compute only the energy in Λ. The most general formula we will ever need is
$$H_\Lambda(S) := \sum_{\substack{A\subset\mathbb{Z}^d \text{ finite} \\ A\cap\Lambda\neq\emptyset}} \Phi_A(S) \tag{2.2}$$
where Φ_A is a function that depends only on S_A. To make everything well defined, we require, e.g., that Φ_A is translation invariant and that $\sum_{A\ni 0} \|\Phi_A\|_\infty < \infty$. (The infinity norm may be replaced by some other norm; in particular, should the need arise to talk about unbounded spins.) It is often more convenient to write the above as a formal sum:
$$H(S) := \sum_A \Phi_A(S) \tag{2.3}$$
with the above specific understanding whenever a precise definition is desired.

The energy is not sufficient on its own to define the statistical mechanics of such spin systems; we also need to specify the *a priori measure* on the spins. This will be achieved by prescribing a Borel measure μ_0 on Ω (which may or may not be finite). Before the interaction is "switched on," the spin configurations will be "distributed" according to the product measure, i.e., the *a priori* law of S_Λ is $\bigotimes_{x\in\Lambda} \mu_0(\mathrm{d}S_x)$. The full statistical-mechanical law is then given by a *Gibbs measure* which (in finite volume) takes the general form $\mathrm{e}^{-\beta H(S)} \prod_x \mu_0(\mathrm{d}S_x)$; cf Sect. 2.3 for more details.

2.2 Examples

Here are a few examples of spin systems:

(1) *$O(n)$-model*: Here $\Omega := \mathbb{S}^{n-1} = \{z \in \mathbb{R}^n : |z|_2 = 1\}$ with $\mu_0 :=$ surface measure on $\mathbb{S}^{n-1}$. The Hamiltonian is

$$H(S) := -J \sum_{\langle x,y\rangle} S_x \cdot S_y \tag{2.4}$$

where the dot denotes the usual (Euclidean) dot-product in $\mathbb{R}^n$ and $J \geq 0$. (Note that this comes at no loss as the sign of J can be changed by reversing the spins on the odd sublattice of $\mathbb{Z}^d$.)

Note that if $A \in O(n)$ — i.e., A is an n-dimensional orthogonal matrix — then

$$AS_x \cdot AS_y = S_x \cdot S_y \tag{2.5}$$

and so $H(AS) = H(S)$. Since also $\mu_0 \circ A^{-1} = \mu_0$, the model possesses a *global rotation invariance* — with respect to a simultaneous rotation of all spins. (For $n = 1$ this reduces to the invariance under the flip $+1 \leftrightarrow -1$.)

Two instances of this model are known by other names: $n = 2$ is the *rotor model* while $n = 3$ is the (classical) *Heisenberg ferromagnet.*

(2) *Ising model*: Formally, this is the $O(1)$-model. Explicitly, the spin variables σ_x take values in $\Omega := \{-1, +1\}$ with uniform *a priori* measure; the Hamiltonian is

$$H(\sigma) := -J \sum_{\langle x,y\rangle} \sigma_x \sigma_y \tag{2.6}$$

Note that the energy is smaller when the spins at nearest neighbors align and higher when they antialign. (A similar statement holds, of

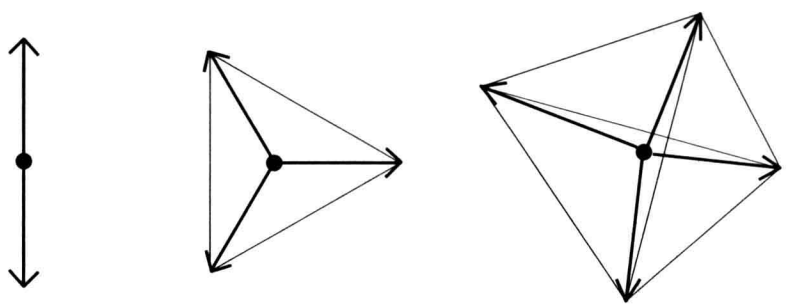
course, for all $O(n)$ models.) This is due to the choice of the sign $J \geq 0$ which makes these models *ferromagnets*.

(3) *Potts model*: This is a generalization of the Ising model beyond two spin states. Explicitly, we fix $q \in \mathbb{N}$ and let σ_x take values in $\{1, \dots, q\}$ (with a uniform *a priori* measure). The Hamiltonian is

$$H(\sigma) := -J \sum_{\langle x,y \rangle} \delta_{\sigma_x, \sigma_y} \tag{2.7}$$

so the energy is $-J$ when σ_x and σ_y "align" and zero otherwise. The $q = 2$ case is the Ising model and $q = 1$ may be related to bond percolation on $\mathbb{Z}^d$ (via the so called *Fortuin-Kasteleyn representation* leading to the so called *random-cluster model*).

It turns out that the Hamiltonian (2.7) can be brought to the form (2.4). Indeed, let Ω denote the set of q points uniformly spread on the unit sphere in $\mathbb{R}^{q-1}$; we may think of these as the vertices of a q-simplex (or a regular q-hedron). The cases $q = 2, 3, 4$ are depicted in this figure:



More explicitly, the elements of Ω are vectors $\hat{\mathrm{v}}_\alpha$, $\alpha = 1, \dots, q$, such that

$$\hat{\mathrm{v}}_\alpha \cdot \hat{\mathrm{v}}_\beta = \begin{cases} 1, & \text{if } \alpha = \beta, \\ -\frac{1}{q-1}, & \text{otherwise.} \end{cases} \tag{2.8}$$

The existence of such vectors can be proved by induction on q. Clearly, if S_x corresponds to σ_x and S_y to σ_y, then

$$S_x \cdot S_y = \frac{q}{q-1} \delta_{\sigma_x, \sigma_y} - \frac{1}{q-1} \tag{2.9}$$

and so the Potts Hamiltonian is to within an additive constant of

$$H(S) := -\tilde{J} \sum_{\langle x,y \rangle} S_x \cdot S_y \tag{2.10}$$

with $\tilde{J} := J\frac{q-1}{q}$. This form, sometimes referred to as *tetrahedral representation*, will be far more useful for our purposes than (2.7).

(4) *Liquid-crystal model*: There are many models that describe certain granular materials known to many of us from digital displays: liquid crystals. A distinguished feature of such materials is the presence of *orientational long-range order* where a majority of the grains align with one another despite the fact that the system as a whole is rotationally invariant. One of the simplest models capturing this phenomenon is as follows: Consider spins $S_x \in \mathbb{S}^{n-1}$ with a uniform *a priori* measure. The Hamiltonian is

$$H(S) := -J \sum_{\langle x,y \rangle} (S_x \cdot S_y)^2 \tag{2.11}$$

The interaction features global rotation invariance and the square takes care of the fact that reflection of any spin does not change the energy (i.e., only the *orientation* rather than the *direction* of the spin matters).

As for the Potts model, the Hamiltonian can again be brought to the form reminiscent of the $O(n)$-model. Indeed, given a spin $S \in \mathbb{S}^{n-1}$ with Cartesian components $S^{(\alpha)}$, $\alpha = 1, \ldots, n$, define an $n \times n$ matrix Q by

$$Q_{\alpha\beta} := S^{(\alpha)} S^{(\beta)} - \frac{1}{n}\delta_{\alpha\beta} \tag{2.12}$$

(The subtraction of the identity is rather arbitrary and more or less unnecessary; its goal is to achieve zero trace and thus reduce the number of independent variables characterizing Q to $n-1$; i.e., as many degrees of freedom as S has.) As is easy to check, if $Q \leftrightarrow S$ and $\tilde{Q} \leftrightarrow \tilde{S}$ are related via the above formula, then

$$\mathrm{Tr}(Q\tilde{Q}) = (S \cdot \tilde{S})^2 - \frac{1}{n} \tag{2.13}$$

Since Q is symmetric, the trace evaluates to

$$\mathrm{Tr}(Q\tilde{Q}) = \sum_{\alpha,\beta} Q_{\alpha\beta}\tilde{Q}_{\alpha\beta} \tag{2.14}$$

which is the canonical scalar product on $n \times n$ matrices. In this language the Hamiltonian takes again the form we saw in the $O(n)$ model.