Theoretical and Mathematical Physics

Scaling Limits in Statistical Mechanics and Microstructures in Continuum Mechanics

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Preface

I began this book about eight years ago after Antonio De Simone, Stephan Luckhaus and Stefan Müller asked me to give a series of lectures on statistical mechanics at the Max Planck Institute in Leipzig. I wrote some notes and after many attempts to make them more readable a book finally came out.

The way a continuum description emerges from atomistic models is an intriguing and fascinating subject, which is behind most of my scientific life, in particular the analysis of large scale phenomena in statistical mechanics and their mathematical formulation in terms of thermodynamic and hydrodynamic limits. The theory has remarkably progressed in the last decades with contributions from many different areas of mathematics and physics, and when asked to give in Leipzig an overview of the state of the art I accepted with great pleasure.

There is the reverse direction as well, where starting from a continuum description after successive blow-ups we find microstructures and the prodromes of an underlying microscopic world. Even though the two directions from microscopics to macroscopics and vice versa are in principle symmetric, mathematical techniques and ideas have proceeded quite separately. I discovered during my lectures that there was a great interest in the audience, whose background was mostly in analysis and continuum mechanics, to learn methods and procedures of statistical mechanics. At the same time it became clear to me that notions and theories developed in continuum mechanics and PDEs had direct implications on my research in statistical mechanics and, to state it succinctly, I felt excited by the idea of building bridges between the two areas, and this book is certainly part of such efforts. Since the book is meant for both communities, it is written with the presumption that the readers may not be expert on all topics; thus the analysis starts from the beginning with parts which are rather elementary and open to younger researchers entering in the field. Statistical mechanics is exemplified in Part I of the book in the context of the Ising model, to avoid technical problems about unboundedness of the variables. Part II is devoted to the mesoscopic theory, which is presented by studying a non-local version of the classical scalar Ginzburg–Landau functional, namely the L–P free energy functional introduced by Lebowitz and Penrose in their analysis of Kac potentials. Part III is more specialistic; it shows how variational methods characteristic of the mesoscopic theory can be used to implement the Pirogov–Sinai theory of phase transitions in lattice and continuum models with Kac potentials.

The choice of working on particular models (Ising, the L–P functional) reflects the didactic purposes of the presentation as well as the taste of the author. I have used parts of the book for lectures in schools and for theses. The various topics can be easily singled out to be used for courses or lectures as I have tried to make the parts not too strongly correlated. Chapter 1 is an introduction essentially based on some survey lectures I gave in the last years, and it hopefully gives a first idea of flavor and content of the book, without entering into too many details.

Part I is about the statistical mechanics of the Ising model. Besides the basic elements of the theory I have also included a more advanced part on the structure of the DLR (Dobrushin, Lanford and Ruelle) measures as a corollary of the Rohlin theory of conditional probabilities for Lebesgue measures, which is explained in some detail. This is a very beautiful and instructive piece of mathematics; it has been fundamental in my education, and for this reason I am fond of it and felt that I had to insert it in the book. Using the theory of DLR measures as a technical tool, I have then shown how the Boltzmann hypothesis that the entropy is proportional to the log of the number of states allows one to derive the thermodynamic potentials. With the help of DLR theory, it is possible to implement Cramer's large deviation methods to prove the existence of the thermodynamic potentials. This is not the traditional way followed in statistical mechanics, but it has the advantage to underline connections with other fields like probability and information theory. All this is in Chap. 2. With Chap. 3 begins the analysis of phase transitions. Still, in the context of the Ising model I discuss here the basic theorems about existence and non-existence of phase transitions, in particular the "Peierls argument" and the "Dobrushin uniqueness theorem," which have fundamental importance in the whole book. Chapter 4 is about mean field and Kac potentials; here scalings, coarse graining and free energy functionals appear for the first time: this is the beginning of the bridge towards mesoscopic and continuum theories. Chapter 5 is about stochastic dynamics; it is in a sense a detour from the main line, but dynamics enters too much into the microscopic and macroscopic theories that I could not leave it completely out of the book. To give a flavor of the research in this field I have presented a derivation of the macroscopic limit evolution for Glauber dynamics with Kac potentials, but I have also inserted a still elementary part where stochasticity persists in the limit, discussing spinodal decomposition and tunneling for the mean field interaction.

Part II is devoted to the mesoscopic theory. For readers whose main interest is in continuum mechanics this could be where to start the book with a "smooth introduction towards statistical mechanics." The presentation is in fact self-contained; motivations for the choice of the free energy functionals come from statistical mechanics, but if the reader accepts the functionals as primitive notions, then references to Part I are not necessary. Chapter 6 starts with a derivation of the thermodynamic potentials, which, in the context of the mesoscopic theory, amounts to the study of some variational problems with constraints. The analysis parallels the one in Chap. 2 for the Ising model and it is certainly instructive to see the two in perspective. I then consider dynamics studying a non-local version of the Allen–Cahn equation related to the L–P free energy functional. As in reaction–diffusion equations, properties like the "Barrier Lemma" and the Comparison Theorem are proved. They are then used to study "large deviations" which, in the mesoscopic theory, refer to estimates of the free energy cost of excursions away from equilibrium. Here contours are introduced and Peierls estimates are proved, in analogy with the corresponding notions and results in the Ising model. As mentioned before, this chapter could be seen as an introduction to statistical mechanics and Part I could be read right after this. In Chap. 7 a first application of large deviation estimates are presented by studying surface tension and Wulff problems for the L–P functional. The basic notions here are Gamma convergence and geometric measure theory, which in fact play a fundamental role; yet some of their basic theorems are here recalled without proofs. In the original plan of the book I had in mind to insert in Part III the statistical mechanics analogue in the context of the LMP particle model introduced by Lebowitz, Mazel and Presutti to study phase transitions in the continuum, but the book was already too long and I gave up. Chapter 8 concludes the analysis of the surface tension for the L–P free energy functional with the study of the shape of the interface (instanton) in the one dimensional case. The instanton is the minimizer of the free energy over profiles constrained to approach the plus and minus equilibrium values at plus and minus infinity, it is therefore a blow up of the interface between the two equilibrium phases. Existence and properties of the instanton including the dynamical ones are proved in this chapter; in particular, spectral gap estimates in a L^∞ setting using an extension of the Dobrushin uniqueness theory of Chap. 3, which involves Vaserstein distance and couplings. I had also planned a chapter about motion by curvature but dropped it for reasons of space (maybe next time…).

Part III is more specialistic, and it has been written with several aims. One was to show how ideas and methods of the mesoscopic theory can find applications in statistical mechanics. Chapter 9 shows that the large deviation estimates of Chap. 6 for the L–P functional can be used to prove the Peierls estimates in the Ising model with ferromagnetic Kac potentials and hence the occurrence of phase transitions in $d \geq 2$ dimensions. I like the result, because it gives an example of the power of Kac ideas in implementing the van der Waals theory of liquid–vapor phase transitions. The careful analysis of the L–P functional in Part II allows one to carry out the Kac program without actually taking the scaling limit as $\gamma \to 0$ (range of the interaction to infinity) and it shows that the mean field phase diagram is a good approximation of the true phase diagram if γ is small. Coarse graining, block spins, effective hamiltonian, and renormalization group ideas appear naturally at this stage. For brevity I do not discuss the specific structure of DLR measures also because they are examined in Chaps. 11 and 12 in the more complex context of the LMP model. The analysis of the Ising model is made simple by the spin flip symmetry, which maps the minus and plus phases one into the other. The Pirogov–Sinai theory is an important step in statistical mechanics which provides methods for deriving Peierls estimates on contours when the symmetry is absent. The original theory was designed to study perturbations of the ground states at small positive temperatures and my purpose in the book is to discuss how the theory can be adapted to study perturbations of the minimizers of the free energy functional at small γ. Instead of adding terms to the Ising hamiltonian to break the spin flip symmetry I have thought it more informative to consider the LMP particle model. This is a system of point particles in $\mathbb{R}^d$ which interact via Kac potentials and which in its mean field approximation has a phase transition into a plus and a minus state with distinct particle densities. There is no symmetry between the two phases and the analysis of the small γ perturbations of the minimizers requires the use of the Pirogov–Sinai theory, which is presented in all detail in Chaps. 10 and 11. In Chapter 12 I have added a characterization of the DLR measures for the LMP model which is not in the existing literature. For reasons of space I have dropped the derivation of the Gibbs phase rule in LMP, for which

I refer to the literature. At the end of Parts I, II and III there are short sections with references and notes. In the subject index the reader will find a list of the most used symbols.

Even though I appear as the author of the book I am certainly not the only one. All this is the outcome of many discussions with friends and colleagues, and parts are taken from lectures and then modified with the help and the comments of the audience. I have just tried to reorganize all that, and the result therefore is not only mine. In particular, the program to study Kac potentials keeping the scaling parameter γ fixed was originally conceived and then carried out with Marzio Cassandro to whom I am especially indebted. Dynamics and its macroscopic limits are instead mostly related to my works with Anna De Masi who also helped me a lot in writing this book. Giovanni Bellettini explained to me some of the fascinating ideas of De Giorgi and helped me to approach the subject from the side of the macroscopic theory.

The influence of the Moscow school is evident in the book and more generally in the way mathematical physics looks today, which is, I believe, largely due to the contributions of the Soviet school and this obviously reflects in the book where the names of Dobrushin and Sinai are recurrent. I learned a lot from them and not only mathematics. There are topics which are not yet ready, in particular a whole big chapter about elastic bodies where there are some intriguing ideas of Stephan Luckhaus which we are trying to develop. But this is for the future and I would like to conclude this preface by mentioning Joel Lebowitz who has been for me a teacher and a friend and if there is something good in this book the credit is certainly his.