Theoretical and Mathematical Physics

The series founded in 1975 and formerly (until 2005) entitled *Texts and Monographs in Physics* (TMP) publishes high-level monographs in theoretical and mathematical physics. The change of title to *Theoretical and Mathematical Physics* (TMP) signals that the series is a suitable publication platform for both the mathematical and the theoretical physicist. The wider scope of the series is reflected by the composition of the editorial board, comprising both physicists and mathematicians.

The books, written in a didactic style and containing a certain amount of elementary background material, bridge the gap between advanced textbooks and research monographs. They can thus serve as basis for advanced studies, not only for lectures and seminars at graduate level, but also for scientists entering a field of research.

Errico Presutti

Scaling Limits in Statistical Mechanics and Microstructures in Continuum Mechanics

With 23 Figures

Springer

Professor Errico Presutti
Dipartimento di Matematica
Università di Roma Tor Vergata
Via della Ricerca Scientifica 1
00133 Roma
Italy
presutti@mat.uniroma2.it

ISBN 978-3-540-73304-1 e-ISBN 978-3-540-73305-8

DOI 10.1007/978-3-540-73305-8

Theoretical and Mathematical Physics ISSN 1864-5879

Library of Congress Control Number: 2008933708

Mathematics Subject Classification (2000): 82B26, 49Q20, 74A15

Cover design: eStudio Calamar S.L.

Printed on acid-free paper

9 8 7 6 5 4 3 2 1

springer.com

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 nonlocal 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.

Errico Presutti, *Scaling Limits in Statistical Mechanics and Microstructures in Continuum Mechanics*, © Springer 2009

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.

Contents

Part IV Appendices

Chapter 1
Introduction

Movies in modern theaters have astonishingly realistic effects. While sitting in your chair and watching the movie, you enter into the middle of the action with sounds and images which surround and overwhelm you. Yet, after all, the magic of all that comes from a loss of information. A movie is just a sequence of images (and sounds) and by looking at them one by one, we certainly gather more information than when we watch them running at the right speed. Moreover, each single image can be amplified more and more, with new details revealed at each step, till it turns out to be an array of pixels or grains, which is the ultimate content of the image. But if we analyze the images to such an extent we are very likely to miss the story of the movie, which, after all, is what it was all about.

All that means that each event has its own characteristic scale, and that even though, theoretically, we improve by successive blow-ups, in fact we may be losing the true meaning of the phenomenon. Sometimes, however, atomization is useful; you may for instance remember the movie "Call Northside 77A" (starring James Stewart) with the trick of magnifying the newspaper to read its date, which proved the alibi of the main character of the story. Blow-ups and slow motions are very popular in sport events, revealing for instance a possible off-side or a penalty in a soccer game, which, at normal speed, are easily missed.

If we replace the word "movies" by "fluids" we are not too far from catching the spirit of this book. The transition from statistical mechanics to continuum mechanics requires a perspective view of the system which captures its main global features and, unavoidably, neglects the details. Sometimes, however, the missing details are just those necessary for explaining a phenomenon and the backward way to microscopics becomes necessary.

There are several levels on the way from microscopics to macroscopics, each one with its own primitive notions, basic axioms and a theory developed from them. Scaling limits and blow ups interrelate the different levels, some links are well established, others are only tentative or just missing, yet the theory is overall in a satisfactory enough shape to justify my attempt to write a monograph on the subject. My goal in this introduction is to give a feeling of the general picture. I will be purposely vague, requiring from the reader a great deal of cooperation for tolerance of the missing details. The hope is to reach in a few pages an idea of the spirit of what research is doing in this area. A quantitative analysis of some of the topics will then come in the successive chapters; other issues will not be expanded further and the reader should look in the literature for more information.

A good way to start is to pick up a specific, interesting issue—interfaces and their structure is my choice—and see how it is developed in the various levels.

Errico Presutti, *Scaling Limits in Statistical Mechanics and Microstructures in Continuum Mechanics*, © Springer 2009

1.1 The macroscopic theory

In the macroscopic theory systems are continuum bodies, each point of the body is representative of a microscopic system in thermal equilibrium; namely a "macroscopic point" observed with a "magnifying lens" becomes a fluid in thermodynamic equilibrium. The parameters which characterize the equilibrium are called "order parameters"; they are specified by the thermodynamic properties of the body and are usually finite in number. Hence the basic postulate of the macroscopic theory is that macroscopic states are local equilibrium states described by order parameter valued functions on the spatial domain Ω occupied by the body.

Besides the temperature which in the sequel is kept fixed throughout the whole body (and thus not included among the order parameters) there are other parameters which characterize the equilibrium states of the system. In a gas an order parameter could be the particle or mass density, but the same substance at lower temperatures, when it solidifies, may also be characterized among other things by its crystalline structure, namely the microscopic pattern in which its atoms are arranged. Thus the order parameter may change drastically with the substance or in the same body if we vary the external conditions. To simplify the discussion we restrict ourselves in the sequel to the simplest case of a single, scalar order parameter, and for the sake of definiteness we consider a ferromagnetic crystal in thermal contact with a reservoir which by exchanges of energy keeps each point of the body at a fixed temperature T. As said before, T is fixed and it does not appear as an order parameter. We further simplify the picture by supposing that the magnetization m along some characteristic axis of the body is the only thermodynamically relevant quantity, so that the scalar m is the order parameter of our system. We also suppose that the reservoir exchanges magnetization with the body so that the total magnetization is not a conserved quantity and at equilibrium m will only have finitely many values: if T is larger than the "critical Curie temperature" only one phase exists (the non-magnetized phase) and $m = 0$ is the only equilibrium value. Below the critical temperature there exist magnetized phases, and the simplest case, which is the one considered here, is when m has only two values, which in proper units are ± 1 (recall that the temperature is fixed) and correspond to the "plus" and to the "minus phase."

As mentioned previously the macroscopic states are functions $m(r)$ which in the present scheme become ± 1 valued functions. The constant functions $m(r) \equiv 1$ and $m(r) \equiv -1$ are global equilibria; they describe the plus and the minus phases, respectively. All the other states are non-equilibrium and in the macroscopic theory they are states for which both phases coexist; they are characterized by two distinct regions, Ω_+ and Ω_-, where respectively $m = 1$ and $m = -1$; see Fig. 1.1. The macroscopic theory postulates that the excess free energy $F(m)$ of such a state m (i.e. the difference of the free energy of m and the free energy of either one of the two global equilibrium states, $m(r) \equiv 1$ and $m(r) \equiv -1$, which have the same free energy) concentrates on the "interface" Σ which separates Ω_+ and Ω_-. Supposing Σ to be a regular surface,

$$F(m) = \int_\Sigma s_\beta(\nu(r))\, dH^{d-1}(r), \tag{1.1.1}$$

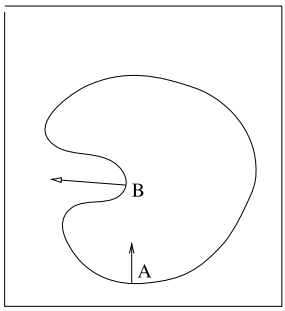

Fig. 1.1 The *thick line* represents the interface between Ω_+ inside and Ω_- outside. The *arrows* are the velocities of A and B under motion by mean curvature: A moves toward the interior, B toward the exterior

where β is "the inverse temperature," more precisely $T = (k\beta)^{-1}$, k the Boltzmann constant; $s_\beta(\nu) > 0$ is the surface tension of a planar interface with unit normal ν, $s_\beta(\nu) = s_\beta(-\nu)$; $\nu(r)$ is the unit normal to Σ at r and dH^{d-1} is the Hausdorff surface measure on Σ.

We can extend (1.1.1) by a limit procedure (for instance in the L^1-sense) to a more general class of states m; the physically acceptable states will be those with bounded free energy, hence the question:

Characterize the states which are limits of regular interface states with bounded free energy. Does the free energy cost of an interface control its regularity?

"Geometric measure theory" gives a full answer to the question. It shows that it is possible to extend the measure of the boundary of a set to "bounded variation," BV, sets, and that, measure theoretically, the boundary of a BV set is almost everywhere C^1 [9, 116]. Thus modulo sets of zero measure we may regard the surface as C^1, and (1.1.1) therefore naturally extends to functions in $BV(\Omega, \{-1, 1\})$, namely functions m such that $\{m = 1\}$ and $\{m = -1\}$ are BV sets. Any other state, which is not BV, has an infinite free energy cost: thus the cost of an interface controls its regularity (in the C^1 sense) but only modulo a region of the interface of zero measure.

Let us now turn to dynamics. Thermodynamics states that the free energy must decrease in time till global equilibrium is established. In agreement with this picture the macroscopic theory postulates that time evolution is defined as the gradient flow of the free energy. The gradient flow of a function $f(r)$, $r \in \mathbb{R}^n$, is defined by the evolution equation $dr(t)/dt = -c\,\nabla f(r(t))$ for $r(t)$, $c > 0$ a constant. Namely the velocity is directed opposite to the gradient. As a consequence f decreases along the orbits, $df/dt = -c|\nabla f|^2$, and in fact the gradient dynamics is often used as a tool to search the minimum of a function.

To apply the above to our case we need to define the gradient of the functional (1.1.1), but we shall discuss this issue in the simpler context of the mesoscopic theory. Here we just say that the gradient flow equation associated to (1.1.1) is motion by curvature. In the isotropic case where the surface tension s_β is independent of the orientation, $s_\beta(\nu) = s_\beta$, this is

$$v(r) = c s_\beta\, \kappa(r)\, \nu(r), \qquad \kappa(r) = \sum_{i=1}^{d-1} \kappa_i(r), \tag{1.1.2}$$

where $v(r)$ is the velocity of the point r of the interface; $c > 0$ a "mobility coefficient"; $\kappa_i(r)$ the i-th principal curvature, counted negative if directed toward the interior, $\nu(r)$ the unit, external normal to the interface at r; in the anisotropic case [203], the principal curvatures are not weighted equally, the weights being determined by the "stiffness matrix." Existence and uniqueness for the Cauchy problem for (1.1.2), is another important chapter of the PDE theory. Existence of classical solutions (i.e. regular moving surfaces which at all points satisfy (1.1.2)) is proved for finite positive times if the initial surface is regular. It is known that singularities may develop after finite times and the continuation of the solution requires the introduction of a weaker notion of solutions; see for instance [117]. Notice finally that by construction the interface area decreases in time and consequently its free energy does so as well, in agreement with the thermodynamic laws.

The basic postulate of the macroscopic theory that each point is representative of a system in thermodynamic equilibrium looks shaky at the interface, where the excess free energy is concentrated and the whole action takes place. Hence the idea of a blow up and of relaxing the local equilibrium postulate of the macroscopic theory, which leads us into the mesoscopic theory.

1.2 The mesoscopic theory

Also, the mesoscopic theory postulates that each point of the body is representative of a portion of fluid; however, unlike in the macroscopic theory, its smaller size allows for deviations from thermodynamic equilibrium. Thus, referring again to the ferromagnetic crystal in thermal contact with a reservoir at a temperature below the critical one, the order parameter will still be the magnetization density m, but now m may take values different from ± 1, which, as before, we suppose to be the equilibrium values.

Thus, a state is now a function $m \in L^\infty(\Lambda, \mathbb{R})$, Λ the region occupied by the body (there is a reason to use Λ instead of Ω, as we shall see). Again $m \equiv 1$ and $m \equiv -1$ are the global equilibrium states and we set as before their free energies equal to 0. Any other state then has a non-zero free energy. The free energy functional in the mesoscopic theory is again a primitive notion. In the scalar Ginzburg–Landau theory it is supposed to have the form

$$F(m) = \int_\Lambda W(m(r)) + |\nabla m|^2, \tag{1.2.1}$$

m being a continuous function with derivative in L^2, $F(m) = +\infty$ on all the other functions. For simplicity we take Λ to be a torus in $\mathbb{R}^d$ (of side L), $W(\cdot)$ a double well potential with two minima at $m = \pm 1$, and elsewhere $W > 0$; to be definite $W(m) = (m^2 - 1)^2/4$.

In the mesoscopic theory the pure phases are defined as the states which minimize the free energy. In (1.2.1) $W(\cdot)$ penalizes excursions from ± 1 and $|\nabla m|^2$ variations of $m(\cdot)$, hence the minimizers of $F(m)$ are the global equilibria $m \equiv 1$ and $m \equiv -1$.

Interfaces arise in states where the two equilibria coexist, but the simple picture of the macroscopic theory where m takes only the values ± 1 is here inadequate, as the free energy $F(m_\pm)$ of any such state is infinite, due to the term $|\nabla m|^2$ in (1.2.1). Let us then relax the requirement that $m = m_\pm$ by only asking that

$$\fint_\Lambda |m - m_\pm| < \zeta, \qquad \fint_\Lambda f = \frac{1}{|\Lambda|}\int_\Lambda f, \tag{1.2.2}$$

where $\zeta > 0$ is an accuracy parameter which will eventually vanish. Calling L the side of the torus Λ, it has been proved that the inf of $F(m)$ under the constraint (1.2.2) grows proportionally to L^{d-1} as $L \to \infty$; it is also known that minimizing sequences differ appreciably from the state $m_\pm$ only in a neighborhood of order 1 of the interface present in $m_\pm$. To make the statement precise, call Ω the unit torus in $\mathbb{R}^d$, $\psi(r) = L^{-1}r$ the map from Λ to Ω and write for any function u on Ω

$$F_L(u) := L^{-d+1} F(u(\psi^{-1}\cdot)), \quad F \text{ as in (1.2.1).} \tag{1.2.3}$$

Explicitly

$$F_L(u) := \int_\Omega \epsilon |Du|^2 + \epsilon^{-1} W(u), \quad \epsilon := \frac{1}{L}. \tag{1.2.4}$$

If $v \in BV(\Omega; \{-1, 1\})$ is a macroscopic state with an interface it is then "natural" to define an upper and a lower free energy of the state v as

$$\lim_{\zeta\to 0} \limsup_{L\to\infty} \inf_{|u-v|_{L^1(\Omega)}<\zeta} F_L(u), \qquad \lim_{\zeta\to 0} \liminf_{L\to\infty} \inf_{|u-v|_{L^1(\Omega)}<\zeta} F_\Lambda(u). \tag{1.2.5}$$

This is an example of De Giorgi's Γ-convergence, a notion extensively studied in the last decades; see for instance [49, 87]. In the particular case we are considering, the two limits in (1.2.5) exist and are equal, and they are given by the macroscopic free energy (1.1.1) with $s_\beta(v) = s_\beta$ independent of v and determined by the potential W [173] by the simple formula

$$s_\beta = \int_{-1}^{1} \sqrt{W(s)}\, ds. \tag{1.2.6}$$

The result (1.2.6) has a nice physical interpretation. Consider the $d = 1$ version of (1.2.1) with $\Lambda = \mathbb{R}$. Then

$$s_\beta = \inf\left\{ F(m), \liminf_{x\to\infty} m(x) > 0; \limsup_{x\to-\infty} m(x) < 0 \right\} = F(\tanh(\cdot)). \tag{1.2.7}$$

The minimizer $x \to \tanh x$ of (1.2.7) is proved to be unique modulo translations and it is called the "instanton." It has also been proved that in the multi-dimensional case if the interface is regular, optimizing functions u are close to the rescaled instanton; i.e. given any point $r_0 \in \Sigma$ consider the line through r_0 along the normal $\nu(r_0)$ to Σ, then on such a line we see (approximately) the one dimensional instanton $\tanh\{L(r - r_0) \cdot \nu(r_0)\}$.

The result gives a positive answer to the questions raised at the end of Sect. 1.1; we have in fact a theory which recovers the macroscopic free energy of any BV state v by taking the macroscopic limit $L \to \infty$, but if more details on the structure of the interface are needed, they can be obtained by keeping L large but fixed. The interface is then called "diffuse" and described by the one dimensional instanton.

Let us now discuss the dynamics. The mesoscopic theory, just like the macroscopic one, postulates that the equations of motion are gradient flows, namely on the torus Λ,

$$\frac{dm}{dt} = -\frac{dF(m)}{dm} = \Delta m - W'(m). \tag{1.2.8}$$

Equation (1.2.8) is a "reaction–diffusion equation" (Δm is the diffusion, $-W'(m)$ the reaction) which is known in the literature as the "Allen–Cahn equation." Existence and uniqueness for the Cauchy problem for (1.2.8) are here well settled questions; the problems present in the motion by curvature arise when we study the macroscopic limit. As seen in the equilibrium theory, when going to macroscopics we shrink space by a factor L^{-1} and since motion by curvature is invariant under parabolic scaling, we scale time as L^2, so that we define on the torus Ω

$$u_L(r,t) := m(Lr, L^2 t), \quad m \text{ a solution of (1.2.8) in } \Lambda. \tag{1.2.9}$$

If $u_L(r,0) \to v$ in $L^1(\Omega)$ as $L \to \infty$ and if $v \in BV(\Omega, \{-1,1\})$ with an interface which is regular, then for t small enough $u_L(\cdot,t) \to v(\cdot,t)$ in $L^1(\Omega)$ and $v(\cdot,t)$ solves the motion by the mean curvature equation (1.1.2) without the coefficient cs_β. Convergence in fact extends to longer times and even past the appearance of singularities via the notion of viscosity solutions, but this is beyond the purposes of the present discussion and we just refer to the literature; see also Sect. 8.7.

The mesoscopic derivation of (1.1.2) fixes the value of the mobility coefficient c as $c = 1/s_\beta$. As we are going to see this is in agreement with the Einstein relation [203], which predicts that the same mobility c which appears in the motion by curvature is also the mobility coefficient which appears in the linear response theory, which describes the response of our magnetic system to the driving force produced by an external magnetic field h. h modifies the free energy by an additive term:

$$F_h(m) = \int_\Lambda |\nabla m|^2 + W(m) - hm, \tag{1.2.10}$$

and therefore the new dynamics is $\frac{dm}{dt} = -\frac{dF_h}{dm}$. In $d = 1$ and with $\Lambda = \mathbb{R}$, for all $h > 0$ small enough there are traveling wave solutions, namely pairs $\tilde{m}, V$, such that $m(x,t) := \tilde{m}(x - Vt)$ solves

$$\frac{dm}{dt} = -\frac{dF_h}{dm} = \frac{d^2m}{dx^2} - W'(m) + h. \tag{1.2.11}$$

The mobility coefficient in the linear response theory is then defined as

$$c = \lim_{h \to 0} \frac{V}{h}, \tag{1.2.12}$$

namely the ratio of the response, V, to the driving force h in the linear regime, $h \to 0$. By explicit computation the mobility turns out to be equal to $1/s_\beta$, the same as when deriving (1.1.2).

In conclusion, with the mesoscopic theory we can investigate the structure of the interface observing corrections to the [macroscopic theory] postulate of local equilibrium in a region of thickness $\approx \epsilon = 1/L$ around the interface (in macroscopic units) where a special magnetization pattern described by the instanton shape is observed. Deviations from such a behavior are however observed experimentally; they are due to thermal fluctuations which make the interface much less regular than predicted by the macroscopic and mesoscopic theories. The number of ways an interface of minimal energy may be deformed adds in fact a relevant entropic contribution to the surface tension which is totally missed in the mesoscopic description. For instance (here the discussion may be a little cryptic for the non-expert), such a contribution is critical in the Potts model (a variant of the Ising model with spins which take a finite number of values ≥ 3): the energy contribution to the surface tension is the same at the interface between "ordered–ordered and ordered–disordered" states, but the entropic contribution is larger in the latter case. As a consequence [170]–[159], at the interface between two distinct "ordered states" there appears a layer of the disordered phase, a phenomenon known as "wetting."

1.3 The microscopic theory

By a blow up we move from the mesoscopic into the microscopic world: macroscopic points are now fully resolved, and as we shall see they become large regions containing many atoms. The unit microscopic length is defined so that the inter-atomic distance (of near-by atoms) has the order of unity. To simplify the picture we restrict ourselves to the Ising model. Microscopic states are then functions $\sigma_\Lambda : \Lambda \to \{-1, 1\}$, Λ being a finite subset of $\mathbb{Z}^d$ representing the crystal location. σ_Λ is identified with a sequence in $\{-1, 1\}^\Lambda$ and $\sigma_\Lambda(x)$ describes the state of "the spin" of the crystal sitting at x. As before it is convenient to regard Λ as a torus in $\mathbb{Z}^d$ (to avoid to have to discuss the interaction with the "walls" confining the system). The energy of the configuration σ_Λ, thought of as repeated periodically in $\mathbb{Z}^d$, is taken to be of the form

$$H_\Lambda^{\mathrm{per}}(\sigma_\Lambda) = -\frac{1}{2} \sum_{x \in \Lambda, y \in \mathbb{Z}^d, y \neq x} J(x, y)\sigma_\Lambda(x)\sigma_\Lambda(y), \tag{1.3.1}$$

where the coupling constants $J(x, y) \geq 0$ because (1.3.1) is supposed to describe a ferromagnetic crystal. Indeed if $J(x, y) > 0$, the interaction energy $-J(x, y)\sigma_\Lambda(x)\sigma_\Lambda(y)$ of the two spins at x and y is minimal if the two spins are "aligned," $\sigma_\Lambda(x) = \sigma_\Lambda(y)$. Thus the minimizers of the energy $H_\Lambda^{\mathrm{per}}(\sigma_\Lambda)$, i.e. its ground states, are $\sigma_\Lambda \equiv 1$ and $\sigma_\Lambda \equiv -1$, as in such states any single pair interaction is minimized (this is why ferromagnetic interactions are much easier to study).

Unlike in the macroscopic and mesoscopic theories, however, the states $\sigma_\Lambda \equiv 1$ and $\sigma_\Lambda \equiv -1$ are not the equilibrium states, they are only the ground states, and they minimize the energy while the equilibrium states are those which minimize the free energy, i.e. energy minus $T \cdot S$, T being the temperature, S the entropy. According to Boltzmann the entropy is proportional to the log of the number of states, and this is the input of the theory of equilibrium statistical mechanics. It leads in the end to a description of the equilibrium states as probability measures [on the phase space of the system] given by the "Gibbs formula"; the whole issue will be discussed in Chap. 2. In our Ising model the "Gibbs measures" are

$$G^{\text{per}}_{\beta,\Lambda}(\sigma_\Lambda) := \frac{e^{-\beta H^{\text{per}}_\Lambda(\sigma_\Lambda)}}{Z^{\text{per}}_\Lambda}, \tag{1.3.2}$$

where $\beta = 1/kT$, T the absolute temperature, k the Boltzmann constant, $H^{\text{per}}_\Lambda(\sigma_\Lambda)$ is given by (1.3.1), Z^{per}_Λ, "the partition function," is the normalization factor:

$$Z^{\text{per}}_\Lambda := \sum_{\sigma_\Lambda \in \{-1,1\}^\Lambda} e^{-\beta H^{\text{per}}_\Lambda(\sigma_\Lambda)}. \tag{1.3.3}$$

Here the Gibbs measure should be regarded as a primitive notion (in Sect. 2.3 we will discuss the derivation of these measures from the Boltzmann hypothesis); thus we will take the axiomatic view that the equilibrium state at inverse temperature β is $G^{\text{per}}_{\beta,\Lambda}$ (at least when Λ is large enough, as we are going to argue). To connect with the macroscopic theory we must preliminarily identify the "macroscopic points" in the microscopic setting. We regard our microscopic region Λ as a blow up of the macroscopic region Ω. Call L the length of the side of the torus Λ and associate to any point $r \in \Omega$ the empirical magnetization

$$u_R(\sigma_\Lambda; r) := \frac{1}{|B_R(Lr)|} \sum_{x \in B_R(Lr) \cap \mathbb{Z}^d} \sigma_\Lambda(x), \quad r \in \Omega, \tag{1.3.4}$$

where σ_Λ is periodically extended to the whole $\mathbb{Z}^d$; $B_R(r) = \{r' : |r - r'| \le R\}$ is l ball in $\mathbb{R}^d$ of radius R and center r, $|B_R(r)|$ is its volume.

Equation (1.3.4) associates to any macroscopic point r the ball $B_R(rL)$ which quantifies the interpretation of macroscopic points in Sect. 1.1 as representative of portions of the fluid with many molecules, how many being determined by R. The mathematical validity of the statement follows from Theorem 1 below; hereafter for the sake of simplicity $J(x, y) = J > 0$ if $|x - y| = 1$ and $J(x, y) = 0$ otherwise.

Theorem 1 *In $d \ge 2$ there is $\beta_c > 0$ so that if $\beta \le \beta_c$ then for any $\zeta > 0$ (and with L the side of the torus Λ)*

$$\lim_{R\to\infty} \lim_{L\to\infty} G^{\text{per}}_{\beta,\Lambda}\big(\|u_R(\sigma_\Lambda; \cdot)\|_{L^1(\Omega)} \le \zeta\big) = 1. \tag{1.3.5}$$

If $\beta > \beta_c$ there is $m_\beta > 0$ so that on calling $\mathbf{1}_{m_\beta}$ and $\mathbf{1}_{-m_\beta}$ the functions on Ω constantly equal to m_β and to $-m_\beta$

$$\lim_{R\to\infty}\lim_{L\to\infty} G^{\mathrm{per}}_{\beta,\Lambda}\big(\|u_R(\sigma_\Lambda;\cdot) - \mathbf{1}_{\pm m_\beta}\|_{L^1(\Omega)} \le \zeta\big) = \frac{1}{2}.$$

Thus the states $\mathbf{1}_{m_\beta}$ and $\mathbf{1}_{-m_\beta}$ when $\beta > \beta_c$ and the state $\mathbf{1}_0$ when $\beta \le \beta_c$ are the equilibrium profiles at the inverse temperature β. We have not normalized the magnetizations and we thus have the equilibrium value m_β instead of 1 as in the previous theories. To proceed with the derivation of the macroscopic theory we will use *the second Gibbs hypothesis*, namely that *the free energy of a macroscopic state is equal to $-\beta^{-1}$ times the log of the Gibbs probability of the macrostate*.

Theorem 2 *For any $d \ge 2$ and $\beta > \beta_c$ there is* [*a surface tension*] *$s_\beta(\nu)$, ν ranging among the unit vectors of $\mathbb{R}^d$, so that for any $w \in BV(\Omega, \{-m_\beta, m_\beta\})$,*

$$\lim_{R\to\infty}\lim_{L\to\infty} \frac{1}{L^{d-1}} \log G^{\mathrm{per}}_{\beta,\Lambda}\big(\|u_R(\sigma_\Lambda;\cdot) - w\|_{L^1(\Omega)} \le \zeta\big) = -\beta F(w),$$

where $F(w)$ is as in (1.1.1).

Notice that Theorem 2 applied to the equilibrium states $\mathbf{1}_{m_\beta}$ and $\mathbf{1}_{-m_\beta}$ shows that they have zero free energy, and thus $F(w)$ is actually the *excess free energy of the macrostate w*.

While Theorem 1 has been established long ago and has been extended to more general lattice systems, Theorem 2 is much more recent. The first paper in $d = 2$ and for β large is the now famous paper [112] by Dobrushin, Kotecký and Shlosman which started the rigorous statistical mechanics theory of interfaces. Interfaces in [112] are actually studied in a much stronger topology than the L^1 norm used in Theorem 2. The results described in Theorem 2 are more recent; they exploit the L^1 context and are based on the geometric measure theory developed in the macroscopic theory; see for instance [39, 76] and references therein.

Interface fluctuations are hidden in the surface tension in Theorem 2; to make them explicit let us fix an "observation window" $B_R(0)$ in the center, say 0, of the cube $\Lambda \subset \mathbb{Z}^d$. To localize the interface we fix plus boundary conditions outside Λ at $x_d > 0$ (the last coordinate of x) and minus boundary conditions at $x_d < 0$, so that a flat interface (as in the mesoscopic and macroscopic theory) would pass through the window and thus be observed. It has been proved [144] that in $d = 2$ if $R = L^a$, $a < 1/2$, then with probability going to 1 the interface does not appear in $B_R(0)$, see Fig. 1.2 while in $d = 2$ and $R = L^a$, $a > 1/2$, as well as in $d = 3$ [108] with any $R(L) \to \infty$ as $L \to \infty$, the interface appears in the window with probability going to 1 as $L \to \infty$, but only if β is larger than a "critical roughness inverse temperature"; see Fig. 1.3.

The actual statistics of the interface fluctuations when the interface is not macroscopically flat are poorly known and this reflects in the essential absence of results in the dynamics of interfaces. The dynamics in the Ising model is defined as a Markov

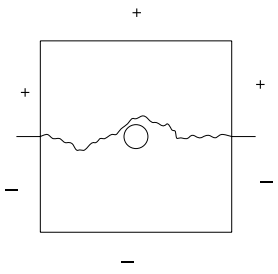

Fig. 1.2 In $d = 2$ and window $B_R(0)$, $R = L^a$, $a < 1/2$

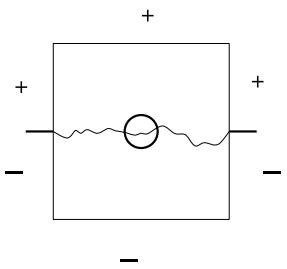

Fig. 1.3 In $d = 2$ and window $B_R(0)$, $R = L^a$, $a > 1/2$ or in $d = 3$ with any $R(L) \to \infty$

process, the Glauber dynamics or the Kawasaki dynamics when the total magnetization is conserved; see Chap. 5. Convergence of the Glauber dynamics to motion by curvature is an open question. Partial results have been obtained in $T = 0$ [202]; for some so called SOS models (where the interface is a graph) [127]; for Kac potentials in some scaling limits [91, 152].

1.4 Kac potentials and the mesoscopic limit

In the previous sections we have seen how and to what extent the macroscopic theory can be derived from an "underlying" mesoscopic or microscopic theory in the scaling limit where the domain Λ invades the whole space. The connection between micro and meso is instead totally missing in the analysis of Sect. 1.3 and indeed it comes from the existence of a third scale which in Sect. 1.3 is not present. There are in principle three main lengths in a system, the inter-atomic distance, which in the Ising model may be taken as the lattice spacing, the interaction range and the size of the spatial domain which defines the macroscopic scale. In Sect. 1.3 we have studied systems where the interaction range is of the same order as the lattice spacing. We have then considered the limit when the region Λ invades the whole space so that the ratio between inter-atomic and macroscopic distances vanishes while the ratio between inter-atomic and effective interaction range stays finite. In this limit the correct thermodynamic behavior emerges and the limit is therefore called "the thermodynamic limit."

There are important examples in physics of long range forces, like the Coulomb and the dipole–dipole interactions, but what we have specifically in mind here are forces à la van der Waals responsible for the liquid–vapor phase transition. Namely

a small but rather long range attractive tail in the interaction which (possibly combined with a short range repulsive force) gives rise to condensation phenomena for suitable values of the density and the temperature. With this in mind we are going to consider systems characterized by having the interatomic and the interaction lengths sharply separated. As discussed in Chap. 4 there are then two possible sub-cases: (i) the interaction and the macroscopic lengths have same order—these are mean field models—and (ii) both ratios, lattice spacing/interaction length and interaction length/macroscopic length vanish; this category contains the Kac potentials which will have a central role in the book. It should be mentioned that also the case where the intermolecular distances are much larger than the range of interaction (the opposite of what we are considering) is of great physical relevance, and by a suitable choice of scales it includes the Boltzmann theory of rarefied gases; see for instance the monograph by Cercignani, Illner and Pulvirenti [75].

We will introduce Kac potentials in the version proposed by Alik Mazel, which has then been used by Lebowitz, Mazel and Presutti in the LMP model; see Chap. 10. Let $\gamma^{-1} \gg 1$ be the mesoscopic length in microscopic units. *The basic assumption is that the energy density $e(\cdot)$ is a function of the empirical magnetization density $u_{\gamma^{-1}}(\sigma_\Lambda; \cdot)$*, namely (after a change of notation)

$$H_{\gamma,\Lambda}(\sigma_\Lambda) = \int_{\mathbb{R}^d} e(J_\gamma * \sigma_\Lambda(r))\, dr \tag{1.4.1}$$

where $J_\gamma * \sigma_\Lambda(r) = \sum_{x\in\mathbb{Z}^d} J_\gamma(x, y)\sigma_\Lambda(y)$ and $J_\gamma(r, r') = \frac{1}{|B_{\gamma^{-1}}|}\, \mathbf{1}_{|r-r'|\le\gamma^{-1}}$ so that $\int J(r, r')dr' = 1$. Observe that for any fixed $\gamma > 0$, $H_{\gamma,\Lambda}(\sigma_\Lambda)$ is a finite range, regular many-body hamiltonian of statistical mechanics. The mesoscopic theory instead requires one to take the limit $\gamma \to 0$, as we are going to see.

Let $m(r)$ be "a mesoscopic magnetization profile" on the torus Λ, $\gamma^{-1}\Lambda$ being its microscopic blow-up (suppose for simplicity that γ^{-1} is an integer). It can then be proved that

$$\lim_{\zeta\to 0}\lim_{\gamma\to 0} -\gamma^d \log G_{\beta,\gamma,\gamma^{-1}\Lambda}\big(\|u_{\gamma^{-1}}(\cdot; \sigma_{\gamma^{-1}\Lambda}) - m(\cdot)\|_{L^1(\Lambda)} \le \zeta\big) =: F(m),$$

where according to "the second Gibbs assumption" $F(m)$ is the free energy of the mesoscopic profile m. It can be shown that

$$\begin{aligned} F(m) &= \int_\Lambda \left\{ e(J * m(r)) - \frac{1}{\beta} S(m(r)) \right\}, \\ J(r, r') &= \frac{1}{B_1(0)|}\, \mathbf{1}_{|r-r'|\le 1}, \end{aligned} \tag{1.4.2}$$

$$S(m) = -\frac{1+m}{2}\log\frac{1+m}{2} - \frac{1-m}{2}\log\frac{1-m}{2}, \tag{1.4.3}$$

and since $e(J * m(r))$ is the energy density, $S(m)$ plays the role of the entropy. In Sect. 4.2 it will be seen that $S(m)$ is related to the log of the number of configurations with magnetization density m, in agreement with the Boltzmann hypothesis.

Suppose now that the energy density is $e(m) = \frac{-m^2}{2}$; then

$$F(m) = \int_\Lambda \left\{ -\frac{1}{2}\, m(r) V * m(r) - \frac{1}{\beta} S(m(r)) \right\}, \quad V = J * J, \tag{1.4.4}$$

which in turns can be rewritten as

$$F(m) = \int_\Lambda \left\{ -\frac{1}{2}\, m(r)^2 - \frac{1}{\beta} S(m(r)) \right\} + \frac{1}{4} \int_\Lambda \int_\Lambda V(r, r') \big(m(r) - m(r')\big)^2. \tag{1.4.5}$$

Interpreting the second term as a non-local version of $|\nabla m|^2$, we recover the basic Ginzburg–Landau functional (1.2.1) with $w(m) = -\frac{m^2}{2} - \frac{1}{\beta} S(m)$, which is indeed a double well if $\beta > 1$. On the other hand, when $e(m) = \frac{-m^2}{2}$ the hamiltonian (1.4.1) becomes

$$H_{\gamma,\Lambda}(\sigma_\Lambda) = -\frac{1}{2} \sum_{x,y \in \Lambda} V_\gamma(x, y) \sigma_\Lambda(x) \sigma_\Lambda(y), \tag{1.4.6}$$

where $V_\gamma(x, y) = \gamma^d V(\gamma x, \gamma y)$. This fits with the original formulation of Kac potentials by Kac, Uhlenbeck and Hemmer [147–149], and then widely studied in statistical mechanics starting from the basic paper by Lebowitz and Penrose, [160]. We will study in Chap. 6 the development of the mesoscopic theory starting from (1.4.5), re-deriving the results stated previously for the Ginzburg–Landau functional.

In Part III of this book, which is of a more specialized nature, we will study Kac potentials keeping γ fixed (but sufficiently small). We will see that phase transitions for systems with Kac potentials can be studied as "perturbations" of the mesoscopic states, or, more precisely, that the Pirogov–Sinai theory used to study the small temperature perturbations of the grounds states of lattice models can be extended to study of the small γ perturbations of the minimizers of the limit non-local mesoscopic functionals. In particular, we will apply such considerations first, as a warm up, to the ferromagnetic Ising model with Kac potentials and then to the LMP model [164], for phase transitions in the continuum.

1.5 Notes for the reader

The book is divided into three parts. At the end of each part there is a short section with Notes and References where I collect the references, which in the text are often omitted. In the subject index I have put some of the most used notation. I just mention here the following one which is often used in the book:

$$\fint_\Delta f(r)\, dr := \frac{1}{|\Delta|} \int_\Delta f(r)\, dr, \tag{1.5.1}$$

where $\Delta \subset \mathbb{R}^d$, $|\Delta|$ being its Lebesgue measure, $f \in L^1(\Delta)$. An analogous notation is used for more general measures. When it is clear from the context I may sometimes drop the measure from the integral and just write $\int_\Delta f$.