THEORY OF SIMPLE GLASSES

This pedagogical and self-contained text describes the modern mean field theory of simple structural glasses. The book begins with a thorough explanation of infinite-dimensional models in statistical physics, before reviewing the key elements of the thermodynamic theory of liquids and the dynamical properties of liquids and glasses. The central feature of the mean field theory of disordered systems, the existence of a large multiplicity of metastable states, is then introduced. The replica method is then covered, before the final chapters describe important, advanced topics such as Gardner transitions, complexity, packing spheres in large dimensions, the jamming transition and the rheology of glasses. Presenting the theory in a clear and pedagogical style, this is an excellent resource for researchers and graduate students working in condensed matter physics and statistical mechanics.

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Exact Solutions in Infinite Dimensions

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Contents

Preface

State of the Art: In Search of a Fully Microscopic Theory of Glasses

Most classical solid state textbooks are almost entirely devoted to crystals, see, e.g., [21]. The main reason is that, while the theory of crystalline solids is fully developed, that of amorphous solids is still very incomplete. As a first approximation, crystals can be understood as perfectly symmetric periodic lattices, around which particles undergo small vibrations. A low-temperature harmonic expansion can then be constructed to obtain the thermodynamic properties in terms of harmonic excitations – i.e., phonons. Defects (mostly dislocations) can then be added to the theory to describe crystal flow (or plasticity) and melting [180, 212]. Crystals are well understood mainly because they can be thought of as small perturbations of a perfectly symmetric lattice, the small parameters being the amplitude of thermal vibrations and the density of defects.

Yet most of the solid matter in nature is not crystalline but amorphous: glasses, foams, pastes, granulars and plastics are but a few examples. These materials are not only ubiquitous but also extremely important for practical, everyday applications. For simplicity, in the rest of this book, we call these materials 'glasses'. Glasses display all kind of anomalies with respect to crystals: in particular, their vibrations cannot simply be understood in terms of plane waves, their flow is not mediated by well defined defects, and their dynamics is extremely complex. Unlike crystals, glasses offer no guiding symmetry principle to construct a microscopic theory, and no natural 'small' parameter can be used to organise a perturbative expansion.

Constructing a complete first-principle theory of glasses has then turned out to be an extremely difficult task. Yet a lot of progress has been made and, recently, several books on glasses written (or edited) by theoretical physicists [37, 53, 168, 357] have appeared. These books are largely devoted to the phenomenology of real (or realistic models of) materials, as known from experiments and numerical simulations, and the theoretical approaches they discuss mostly make use of approximate methods. This is, of course, an excellent idea given the complexity of the problem, and it is typical of theoretical physics.

The aim and style of this book is, however, quite different and, in our opinion, complementary to previous efforts. We discuss here the exact solution of a microscopically well-defined model which, we believe, can be taken as the simplest realistic model of a glass. By 'exact solution', we mean that one is able to compute in a mathematically exact way all the relevant observables of the model. Although the solution is not mathematically rigorous, we argue that it is exact from a theoretical physicist's perspective. We believe, as we discuss in the rest of this preface, that the material presented in this book constitutes a useful first step towards reaching the goal of constructing a complete and fully microscopic theory of glasses.

A Digression on the Structure of Scientific Theories

Let us make a philosophical digression to discuss what we can reasonably expect from a theory of glasses. A convenient definition of a 'scientific theory', given[1] by Lucio Russo in [312, section 1.3], is obtained by requiring the following three properties:

1. Its statements do not concern concrete objects pertaining to the real world but specific abstract mathematical objects.
2. It has a deductive structure: it is made by a few postulates concerning its objects and by a method to derive from them a potentially infinite number of consequences.
3. Its application to the real world is based on a series of 'correspondence rules' between the abstract objects of the theory and those of the real world.

According to Russo, a useful criterion for determining whether a theory has these properties is to check if one can compile a collection of exercises that can be solved within the theory. Solving a problem in the context of the theory is then nothing but an (arbitrarily difficult) 'exercise'.

As an example of this structure we can take Newtonian mechanics, where (1) the abstract objects are point particles interacting via forces, (2) the postulates are minimal but the theory is extremely powerful because from these postulates one can deduce an enormous variety of results, and (3) the point particles of the theory can be put in correspondence with many real-world objects, ranging from atoms to planets, depending on the context in which one wishes to use the theory.[2]

[1] Together with a nice discussion of its limits, that is not reproduced here.
[2] Note that we are nowadays used to this kind of logical structure, which is, however, the result of an extremely long historical process. Even the mathematical definition of 'point' has long been debated [312].

This example highlights that the choice of correspondence rules is extremely delicate. We know very well that atoms and planets are not point particles. They have a complex internal structure, which limits the applicability of the theory, giving rise to important physical phenomena.

'Scientific theories', as defined earlier, are powerful for two main reasons:

(i) Working on two parallel but distinct levels (the mathematical model and the real world) allows for a very flexible reasoning. In particular, one can guarantee the 'truth' of scientific statements by limiting them to the domain of the model.
(ii) The theory can be extended, by using the deductive method and introducing new correspondence rules, to treat situations that were not a priori included in the initial objectives for which the theory was developed.

At the same time, it is important to keep in mind that any 'scientific theory' has a limited utility. In general, it can only be used to model phenomena that are not too 'far' from those that motivated its elaboration. Theories that become inadequate to describe a new phenomenology must, for this reason, be substituted. They remain, however, according to our definition, 'scientific theories', and one can continue to use them in their domain of validity [312].[3] This last statement is particularly important because it reminds us that 'the' theory of a given class of phenomena – e.g., the glass transition – will never exist. Scientific theories are never unique or everlasting. They are models of reality, and there is no problem in using different models of the same phenomenon and in replacing current models with more powerful ones when they are found.

Towards a Scientific Theory of Glasses

The aim of this book is to make some steps in the application of the programme mentioned earlier to the problem of glasses. Let us state from the very beginning that we will not be able here to complete this programme. This book is mainly concerned with steps 1 and 2 – i.e., constructing an abstract mathematical theory that has a deductive structure and describes at least the basic phenomenology of glass formation and of the amorphous solid phase. The difficult problem of establishing a correspondence with the real world is left aside here. We give only hints and references to the literature so that the reader can form their own opinion on the proper correspondence rules and judge the quality of the theory according to their own taste. Another book will have to be written on the subject in the future.

[3] For instance, Newtonian mechanics did not become useless once quantum mechanics was developed, and the fact that it gives incorrect predictions (e.g., the instability of the hydrogen atom) does not mean that it is plain wrong.

We believe that the approach described above has important advantages, mostly based on points *(i)* and *(ii)*. Let us give two examples. Concerning point *(i)*, the problem of glasses is extremely complex and many different theories have been proposed. In the attempt to describe real-world materials, most of these theories make heavy use of approximations, to the point that it often becomes quite difficult to establish whether the statements made by the theory are true even within the logical structure of the theory itself. We instead introduce a simple and solvable mathematical model of glass: a system of Newtonian point particles in the limit of infinite spatial dimensions. Our aim is to discuss the mathematical solution of this model, which is already extremely rich and complex. But, although we believe the solution to be exact, a mathematically rigorous proof of its exactness is still lacking, and we hope that presenting the non-rigorous solution in a clear and aspirationally pedagogical way will help progress towards a rigorous proof. Our statements are limited to this mathematical model, and one is then able to decide whether they are true or false in a well-defined mathematical sense. Concerning point *(ii)*, we will see a spectacular example of its power in Chapter 9. The model, originally designed to describe the liquid and glass phases of atomic materials, also displays a phase transition that can be put in correspondence with the jamming transition of granular materials. Thus, the model shows a potential to unify phenomena (glass and jamming transitions) and materials (atomic glasses, colloidal glasses, granular glasses) that were thought to be somehow distinct.

The main, and very important, drawback of this approach is that the infinite-dimensional limit is quite abstract. Hence, the final step of establishing correspondence rules between the different phases and observables of the abstract model and their real-world counterparts (i.e., real liquids, real glasses, real granular materials) is non-trivial and remains largely open to debate. In granular materials, for example, the role of friction remains to be clarified. If successfully performed, this step would ultimately correspond to constructing a scientific theory of real-world glasses (i.e., to implement step 3), but it requires a lot of additional discussion which goes much beyond the scope of this book. Here, when discussing each specific aspect of the mathematical solution of the model, we limit ourselves to a few hints and references to direct the reader towards real-world phenomena that could potentially be described by this solution. This is done at the end of each chapter, in the Further Reading sections. We do not, however, specify completely the list of phenomena that could be accounted for by such a theory, nor do we try to establish precise correspondence rules between the mathematical model discussed here and real-world objects. Discussing this issue with all the needed details will be part of the follow-up publications to the present book.

Historical Note

The idea of using infinite-dimensional solvable models has been extremely successful in condensed matter, appearing in the context of atomic physics [337], liquids [154, 206], ferromagnetic systems [163] and strongly correlated electrons, where it has led to the celebrated dynamical mean field theory [164]. See also [356] for related ideas in high-energy physics.

In the context of the glass transition, the idea of solving the problem in the infinite dimensional limit was first proposed in [206]. A complete and exact solution of the infinite-dimensional problem was then obtained more recently, in a long series of research articles to which we contributed together with many other colleagues [3, 88, 89, 220, 221, 239, 291, 292, 299]. The methods used in this solution are deeply rooted in the theory of spin glasses [79, 254], using dynamical methods [109, 111] and replica methods [144, 260] specifically developed for the glass problem. These methods were first applied to approximate the behaviour of glasses in finite dimensions [76, 252, 253, 256, 292, 366, 368] before it was realised that they become exact in the infinite-dimensional limit [220, 291]. The phase diagram turns out to be similar to that of a class of spin glass models (Ising p-spin and Potts glasses [79, 160, 170, 171, 203, 204, 207]), which confirms the main assumption behind the random first-order transition (RFOT) theory of the glass transition [205, 208, 357]. The solution also reproduces the essential features of the mode-coupling theory of the glass transition [168], as discussed in [239].

The aim of this book is to collect these results and organise them in a pedagogically coherent way. We did not include here any new material (except for some polishing of the original work), and we do not wish to take any additional credit for the results. The original papers are thus carefully referenced along the book.

Target Audience

This book is written having in mind two distinct types of readers. The first are young students (at the level of the final year of undergraduate studies or at the beginning of their graduate studies). We expect these readers to have no or very little background knowledge of the physics of glasses. Reading this book only requires a basic background in statistical mechanics: the mean field (Landau) approach to phase transitions in magnetic materials and some basics in liquid state theory (as covered, e.g., in [175]). We ask these readers to believe our conjecture that a system of infinite-dimensional atoms can be a good mathematical model of glass and to follow us in the mathematical study of the model. Along the way, they will learn advanced statistical mechanics techniques (e.g., the replica method) as well as many deep concepts that pervade the physics of disordered systems (e.g., long-lived metastable states, complex free energy landscapes, ergodicity breaking). By working out all the calculations in this example, they will learn methods that can be used in many different contexts ranging from spin glasses [254] to optimisation problems [251] and neural networks [10]. However, they will not acquire sufficient background about the phenomenology of glasses and on the many different approaches that are used in their theoretical description. For this purpose, we refer to other existing excellent books and reviews [37, 40, 53, 80, 168, 357].

The second group of readers are experienced researchers working on the physics of glasses. We expect them to be already acquainted with the main physical concepts discussed in the book and to be familiar with the material contained in [37, 40, 53, 80, 168, 357]. Yet we hope that these readers will find here a way to put many different pieces of knowledge into a common perspective. Some of these more experienced readers might also be interested in learning the details of the methods mentioned earlier.

Structure of the Book

The book presents the main logical steps of the derivation of the exact solution of amorphous infinite-dimensional particle systems. All the non-trivial steps are presented, but leaving to the reader some trivial intermediate steps (for which we provide references to the original work). At the end of each chapter, a Summary section is provided to recapitulate the main points discussed in the chapter. The correspondence with real-world objects, as well as the comparison with approximate theories of glasses, is logically separated from the main stream of the book.[4] Some elements are presented in short Further Reading sections at the end of the relevant chapters.

The structure of the book chapters is the following.

- Chapter 1 reviews classical results in the statistical mechanics of infinite-dimensional systems, using the Ising model as a paradigmatic example. The notion of metastability is introduced and discussed.
- Chapter 2 provides a short review of classical results in liquid state theory [175] and then introduces the strategy to solve the thermodynamics of atomic liquids in infinite dimensions.
- Chapter 3 presents the solution of the equilibrium liquid dynamics in infinite dimensions by a series of simple arguments, following Szamel [339].

[4] Except in Chapter 9, where the problem is easier and some discussion of this correspondence is provided in the main text.

The existence of a sharp dynamical glass transition, at which the equilibrium diffusion constant vanishes, is discussed.

- Chapter 4 discusses the central feature of the mean field theory of disordered systems, namely the existence of a large multiplicity of metastable states. The replica method is introduced in this context, following Franz and Parisi [144]. The appearance of metastable states is directly connected to the dynamical arrest of the liquid. The exact expression of the replicated free energy of an atomic system is derived, following the ideas of [220, 299] and the detailed derivation of [59]. From this basic object, the glass phase diagram of two model systems is derived. This chapter also contains the core of the mathematical solution of the model.
- Chapter 5 provides a short compendium of basic notions of replica symmetry breaking (RSB) and the associated ultrametric distribution of states in phase space. This chapter is a review of classical results in spin glass theory [254].
- Chapter 6 discusses RSB effects in the Franz-Parisi construction introduced in Chapter 4. The phase diagram of two simple glass models is derived. The notion of a Gardner transition is introduced, and its physical meaning is discussed using the results of Chapter 5. This chapter reviews results originally presented in [88, 299, 315].
- Chapter 7 introduces another replica scheme due to Monasson [260], which allows one to study a different class of metastable states. The phase diagram of hard spheres is derived and compared with that of Chapter 6. The connection with the Edwards approach to the study of jammed packings is discussed. This chapter reviews results originally presented in [88, 93, 291, 292].
- Chapter 8 introduces the sphere-packing problem. A brief review of mathematical and physical results is provided. It is shown how the results obtained in Chapters 4, 6 and 7 provide insight on this problem. This chapter reviews results originally presented in [240, 291, 292, 325].
- Chapter 9 focuses on the jamming transition. It is explained why jamming is a critical point, and the associated critical exponents are described. The non-trivial scaling form of the RSB equations in the vicinity of jamming is discussed in detail. This chapter presents results originally derived in [88, 89, 91].
- Chapter 10 discusses the response of the glass to an applied shear strain. The elasticity and yielding of the glass are discussed. This chapter presents results originally derived in [58, 298, 299, 346].

The reader has certainly noticed that the title of this book makes explicit reference to the classic *Theory of Simple Liquids* by Hansen and McDonald [175]. Our intention is indeed to apply to glasses the same program that was applied to liquids in the 1960s. The word ‘simple’ refers, here and in [175], to the fact that we only consider the simplest model of liquids and glasses: a collection of classical point particles, modelling atoms. There are, of course, much more complex glass-forming systems (e.g., polymer glasses and network glasses, or anisotropic granular systems like hard ellipsoids), but their description falls beyond the scope of this book.

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