

## SPIN GLASSES AND COMPLEXITY

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# SPIN GLASSES AND COMPLEXITY

Daniel L. Stein and Charles M. Newman

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Summary: "Spin glasses are disordered magnetic systems that have led to the development of mathematical tools with an array of real-world applications, from airline scheduling to neural networks. Spin Glasses and Complexity offers the most concise, engaging, and accessible introduction to the subject, fully explaining what spin glasses are, why they are important, and how they are opening up new ways of thinking about complexity. This one-of-a-kind guide to spin glasses begins by explaining the fundamentals of order and symmetry in condensed matter physics and how spin glasses fit into-and modify-this framework. It then explores how spin-glass concepts and ideas have found applications in areas as diverse as computational complexity, biological and artificial neural networks, protein folding, immune response maturation, combinatorial optimization, and social network modeling. Providing an essential overview of the history, science, and growing significance of this exciting field, Spin Glasses and Complexity also features a forward-looking discussion of what spin glasses may teach us in the future about complex systems. This is a must-have book for students and practitioners in the natural and social sciences, with new material even for the experts"- Provided by publisher.

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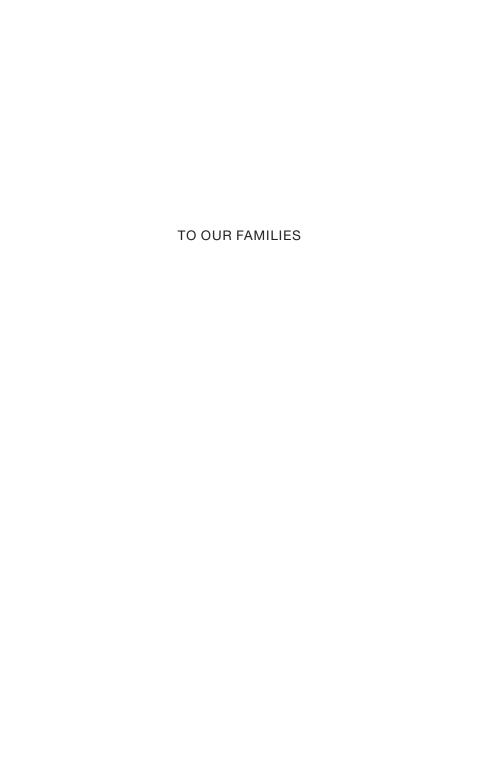
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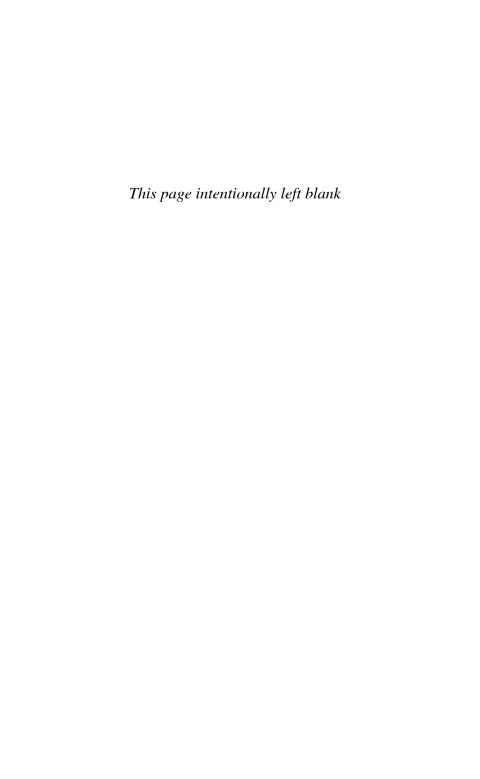
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#### CONTENTS

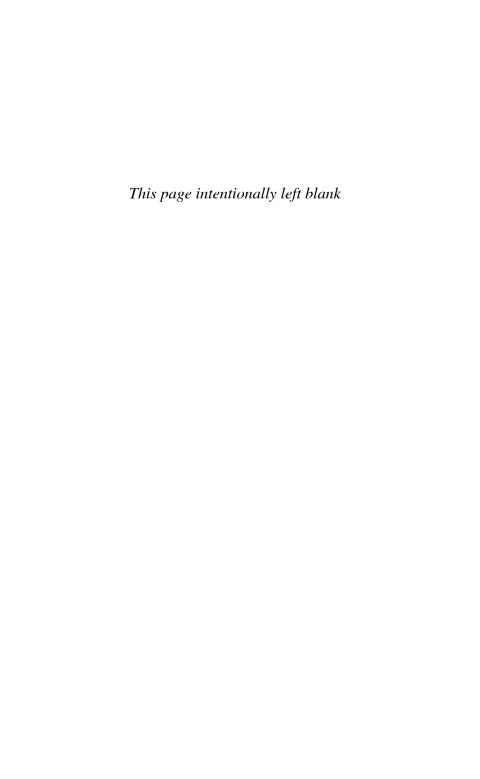
	Preface	X1
	Introduction: Why Spin Glasses?	1
1.	Order, Symmetry, and the Organization of Matter	15
	1.1 The Symmetry of Physical Laws	17
	1.2 The Hamiltonian	23
	1.3 Broken Symmetry	26
	1.4 The Order Parameter	31
	1.5 Phases of Matter	35
	1.6 Phase Transitions	39
	1.7 Summary: The Unity of Condensed Matter Physics	41
2.	Glasses and Quenched Disorder	43
	2.1 Equilibrium and Nonequilibrium	43
	2.2 The Glass Transition	45
	2.3 Localization	49
3.	Magnetic Systems	51
	3.1 Spin	51
	3.2 Magnetism in Solids	53
	3.3 The Paramagnetic Phase	55
	3.4 Magnetization	55

viii Contents

	3.5 The Ferromagnetic Phase and Magnetic	
	Susceptibility	57
	3.6 The Antiferromagnetic Phase	59
	3.7 Broken Symmetry and the Heisenberg Hamiltonian	59
4.	Spin Glasses: General Features	63
	4.1 Dilute Magnetic Alloys and the Kondo Effect	64
	4.2 A New State of Matter?	65
	4.3 Nonequilibrium and Dynamical Behavior	71
	4.4 Mechanisms Underlying Spin Glass Behavior	74
	4.5 The Edwards-Anderson Hamiltonian	78
	4.6 Frustration	81
	4.7 Dimensionality and Phase Transitions	83
	4.8 Broken Symmetry and the Edwards-Anderson Order	
	Parameter	85
	4.9 Energy Landscapes and Metastability	86
5.	The Infinite-Range Spin Glass	90
	5.1 Mean Field Theory	90
	5.2 The Sherrington-Kirkpatrick Hamiltonian	92
	5.3 A Problem Arises	93
	5.4 The Remedy	95
	5.5 Thermodynamic States	97
	5.6 The Meaning of Replica Symmetry Breaking	98
	5.7 The Big Picture	109
6.	Applications to Other Fields	112
	6.1 Computational Time Complexity and	
	Combinatorial Optimization	113
	6.2 Neural Networks and Neural Computation	129
	6.3 Protein Folding and Conformational Dynamics	144
	6.4 Short Takes	168
7.	Short-Range Spin Glasses: Some Basic Questions	175
	7.1 Ground States	177

Contents	ix

	7.2 Pure States	188
	7.3 Scenarios for the Spin Glass Phase of the EA Model	193
	7.4 The Replica Symmetry Breaking and Droplet/Scaling	
	Scenarios	194
	7.5 The Parisi Overlap Distribution	197
	7.6 Self-Averaging and Non-Self-Averaging	199
	7.7 Ruling Out the Standard RSB Scenario	201
	7.8 Chaotic Size Dependence and Metastates	203
	7.9 A New RSB Scenario	206
	7.10 Two More (Relatively) New Scenarios	211
	7.11 Why Should the SK Model Behave Differently from	
	the EA Model?	214
	7.12 Summary: Where Do We Stand?	216
8.	Are Spin Glasses Complex Systems?	218
	8.1 Three Foundational Papers	219
	8.2 Spin Glasses as a Bridge to Somewhere	227
	8.3 Modern Viewpoints on Complexity	228
	8.4 Spin Glasses: Old, New, and Quasi-Complexity	233
	Notes	239
	Glossary	265
	Bibliography	285
	Index	309



#### PREFACE

This book began as a series of lectures given by one of us (DLS) at the 2008 Complex Systems Summer School in Santa Fe, New Mexico. Those lectures were aimed at a broad audience, comprising physicists, mathematicians, biologists, computer scientists, engineers, chemists, economists, and anthropologists, brought together through their interest in the overarching theme of complexity and its relation to their own disciplines.

Presenting a highly technical subject like spin glasses to a diverse set of backgrounds and interests is challenging, to say the least. In retrospect, with our having just finished this book, that earlier challenge seems relatively mild. With a book one can be more expansive and cover more topics, but at the same time one is asked to reach a wider audience, and in some respects the constraints are even tighter. This is, after all, a primer. That means: keep it short, keep it basic, and make sure it's accessible to non-physicists and nonmathematicians. We managed to keep it basic (from the point of view of those working in the field); had a bit more trouble keeping it short, but more or less managed that; and as far as accessibility goes, we can only say that we did our best.

This preface is intended to serve as a guide for the perplexed. Not all of the book needs to be read if you're, say, a biologist xii Preface

who wants to learn a little about the field and its applications to biology. On the other hand, if you're a physicist, you can easily skip the earlier chapters and get right to the good stuff. It won't make you an expert in the field, but it should give you some idea of what it's all about. And, especially in chapter 7, there may be a good deal of new and interesting things—and perhaps a clarification of a number of issues that seem to have retained their fuzziness in the general discourse.

But we want to emphasize that this book is intended to be neither an in-depth study of any topic nor a broad survey. At the same time, perhaps unusual for a primer, it's not simply a collection of selected topics, either; it's been organized along a narrative thread, so that it tells a certain story.

Who should read this book? As noted, it's written for a wide audience of scientists and social scientists interested in complexity science. But at the same time, we've included topics that may be of interest if you don't care at all about (or for) modern-day complexity research but do want to understand some current issues in spin glass research. Given the need for brevity, we can broach only a small subset of the many outstanding problems, but those included do reside at the heart of the current debate regarding the nature of spin glasses.

We've tried to aim the book at a level between that of *Scientific American* and the technical literature. We've assumed the reader has an introductory college-level mathematics background, including one semester of basic calculus and some elementary probability (knowing the meaning of a random variable and its associated probability distribution is sufficient). Even so, we've gone fairly easy on the math, and equations have intentionally been kept few and far between. We don't presume that the reader is very knowledgeable about physics: we guess that most readers will have had physics back in high school and forgotten most of it. If you sort of remember Newton's laws of motion, a little

Preface xiii

basic circuit theory, and some elementary thermodynamics, you should be able to get a good deal out of it. Finally, we've assumed a passing acquaintance<sup>1</sup> with a smattering of topics—chaos, adaptation, emergence—that pervade much of modern complexity research.

#### Outline of the Book

Even without considering applications to biology, computer science, and other areas outside physics, the field of spin glasses is very broad. Numerous technical books and review articles have been written that provide an expansive overview of the subject; this primer is very emphatically not another one.<sup>2</sup> Its focus is deliberately narrow and is largely confined to the equilibrium properties of classical spin glasses. This means that some of the most interesting and recent topics are necessarily omitted, including quantum spin glasses in their entirety, much (but not all) of the work on nonequilibrium dynamics and aging, non-Ising models, related disordered systems (e.g., random field magnets, dipole glasses, random-bond ferromagnets, periodically frustrated systems), and much else.

Our own, undoubtedly idiosyncratic, take on the subject of spin glasses proper is strongly guided by how they both sharpen and challenge the foundations of the edifice, painstakingly built up over many years, of order, symmetry, and broken symmetry in condensed matter systems. The theme of broken symmetry runs through this book and ultimately ties in to questions of complexity and how spin glasses fit into that framework. We emphasize that one needn't worry about these philosophical underpinnings to grasp how spin glass ideas have carried over to other complex systems. But given the unsettled state of the meanings of "complexity" and "complex system," adopting some philosophical point of view is unavoidable. Certainly, plenty of room for disagreement remains, but at least let's try to have some fun.

xiv Preface

In the introduction, we provide an overview of why spin glasses might be of interest to you if you're not a physicist but are interested in any of a variety of other problems outside physics, or more generally in the field of complexity itself. Chapter 1 introduces the basic concepts and language that will be needed later on: order, symmetry, invariance, broken symmetry, Hamiltonian, condensed matter, order parameter, ground state, and several thermodynamic terms.<sup>3</sup> We also present the necessary concepts from thermodynamics and statistical mechanics that will be needed later. Here we boil down the latter to its most elemental and essential ingredient: that of temperature as controlling the relative probabilities of configurations of different energies. For much of statistical mechanics, all else is commentary. This is sufficient to present an intuitive understanding of why and how matter organizes itself into different phases as temperature varies, and leads to the all-important concept of a phase transition.

Chapter 2 immediately challenges some of the notions of chapter 1 by introducing the first of our systems with quenched disorder, namely, ordinary glasses. This requires an explanation of the central notions of equilibrium and nonequilibrium. We can already begin to see how large a gap remains in our understanding of the condensed state, and how powerful is the challenge to conventional statistical mechanics presented by quenched disorder.

Chapter 3 introduces the reader to the basics of solid state magnetism, starting with the quantum mechanical property of spin, and showing how the familiar phenomenon of ferromagnetism—as well as the less familiar but equally important ones of antiferromagnetism and paramagnetism—arises. This is a necessary prelude to understanding the idea of what a spin glass *is*; and so spin glasses finally enter the picture in chapter 4. Here we discuss some of the history of their discovery,

Preface xv

their basic properties and experimental phenomenology, and some of the mysteries surrounding them. We introduce some of the basic theoretical constructs that underlie much of the discussion in later chapters, including the Edwards-Anderson Hamiltonian and order parameter, frustration, metastability, and rugged energy (or free energy) landscapes.

The next chapter introduces the reader to mean field theory, both as a general class of models and in its specific incarnation in spin glasses, the Sherrington-Kirkpatrick model. This is undoubtedly the most theoretically studied spin glass model by far, and the best understood. For the nonphysicist the going may get a little heavy here once replica symmetry breaking is introduced, with its attendant features of many states, non-self-averaging, and ultrametricity—but we define and try to explain what all of these things mean and why replica symmetry breaking represents such a radical departure from more conventional and familiar modes of symmetry breaking. While this is a central part of the story of spin glasses proper, we nevertheless note in the text that the nonphysicist who wants to skip the technical details can safely omit sections 5.3 through 5.6 and continue on without losing the essential thread of the discussion that follows. Physicists, on the other hand, can safely skip everything before chapter 4.

Chapter 6 describes what might be called "old complexity" (with regard to spin glasses). Here we explore how spin glass concepts have found use in and, in some cases, further advanced areas such as computational complexity, combinatorial optimization, neural networks, protein conformational dynamics and folding, and computer science (through the introduction of new heuristic algorithms such as simulated annealing and neural-based computation, and through new approaches to analyzing hard combinatorial optimization problems). We also introduce some "short takes" on topics that space constraints prevent covering in detail but that we felt should be at least mentioned: prebiotic

xvi Preface

evolution, Kauffman's *NK* model, and the maturation of the immune response.

This chapter summarizes the heart of what most people mean when they refer to spin glasses as relevant to complexity. We do not attempt to cover all applications, or even most. Nor, in the topics that we choose, do we attempt to cover the entire body of work on the subject. Instead we focus on the early, classic papers in each subject, giving the reader a flavor of each. More current work in these areas is only sparsely and briefly mentioned, but we hope this chapter provides some basis for further investigation of any of these areas if the reader so desires.

Chapter 7 discusses short-range spin glasses. It is necessary for completeness, but could be skipped on a first reading if you're not a mathematician or a physicist, unless you're really, really interested in the systems themselves.

The study of short-range spin glasses is still evolving, and beset by controversy. It's also a highly technical subject. Again, we've tried to make it user-friendly (including translations from technical jabber into English at various points), but it's likely to be heavy going for most readers. The good news, as we noted, is that you can skip the chapter completely if you don't want to get too deep into the subject. If you do skip most of this chapter, you can still find the main ideas summarized in sections 7.11 and 7.12. But we hope that the persistent reader who takes the plunge will be rewarded.

The focus of the chapter is narrow: its sole concern is the nature of the broken symmetry and order parameter of a spin glass phase—if it exists. It is written unabashedly from a particular point of view. But we try to make clear which parts constitute our own opinion, as well as to present competing points of view. Perhaps unusually, we focus more on analytical than on numerical results, discussing what replica symmetry breaking means—and doesn't mean—for short-range spin glasses, and

Preface xvii

we introduce other scenarios such as droplet/scaling, chaotic pairs, and TNT (trivial link overlap, nontrivial spin overlap). We also present new tools and concepts, such as metastates and chaotic size dependence, and refer to other fundamentally important concepts such as temperature chaos, coupling chaos, and stochastic stability.

The final chapter brings us back to complexity and how spin glasses fit in. We discuss three landmark papers in the field of complexity, by Warren Weaver, Herb Simon, and Phil Anderson, respectively, and examine how the ideas they introduced might relate to our current understanding of spin glasses. We also take a brief look at recent developments, in particular various proposals for measures of complexity, and consider how they might illuminate some features of spin glasses. We close by asking whether spin glasses can still be thought of as "complex systems," and in so doing introduce a proposal for a kind of "new complexity" as it relates to spin glasses.

#### Happy reading.

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xviii Preface

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#### INTRODUCTION: WHY SPIN GLASSES?

Spin glasses are disordered magnetic materials, and it's hard to find a less promising candidate to serve as a focal point of complexity studies, much less as the object of thousands of investigations. On first inspection, they don't seem particularly exciting. Although they're a type of magnet, they're not very good at being magnetic. Metallic spin glasses are unremarkable conductors, and insulating spin glasses are fairly useless as practical insulators. So why the interest?

Well, the answer to that depends on where you're coming from. In what follows we'll explore those features of spin glasses that have attracted, in turn, condensed matter and statistical physicists, complexity scientists, and mathematicians and applied mathematicians of various sorts. In this introduction, we'll briefly touch on some of these features in order to (we hope) spark your interest. But to dig deeper and get a real sense of what's going on—that can fill a book.

## Spin glass research provides mathematical tools to analyze some interesting (and hard) real-world problems.

Suppose you're given the following easily stated problem. You're shown a collection of *N* points on the plane, which we'll call cities. You're asked to start at one of the cities (any one will

2 Introduction

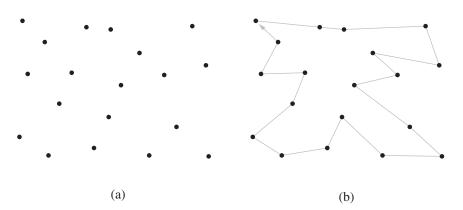


Figure I.1. (a) An instance of a TSP problem with 19 cities. (b) One possible tour.

do), draw an unbroken line that crosses each of the other cities exactly once, and returns to the starting point. Such a line is called a tour, and an example is shown in figure I.1. All you need to do is to find the shortest possible tour.

This is an example of the Traveling Salesman Problem, or TSP for short. An "instance," or realization of the problem, is some specific placement of points on the plane (which a priori can be put anywhere). You should be able to convince yourself that the number of distinct tours when there are N cities is (N-1)!/2. The factor of two in the denominator arises because a single tour can run in either direction.

Notice how quickly the number of tours increases with N: for 5 cities, there are 12 distinct tours; for 10 cities, 181,440 tours; and for 50 cities (not unusual for a sales or book tour in real life), the number of tours is approximately  $3 \times 10^{62}$ . The seemingly easy (i.e., lazy) way to solve this is to look at every possible tour and compute its length, a method called exhaustive search. Of course, you're not about to do that yourself, but you have access

to a modern high-speed computer. If your computer can check out—let's be generous—a billion tours every second, it would take it  $10^{46}$  years to come up with the answer for a 50-city tour. (For comparison, the current age of the universe is estimated at roughly  $1.3 \times 10^{10}$  years.) Switching to the fastest supercomputer won't help you much. Clearly, you'll need to find a much more efficient algorithm.

Does this problem seem to be of only academic interest? Perhaps it is,<sup>2</sup> but the same issues—lots of possible trial solutions to be tested and a multitude of conflicting constraints making it hard to find the best one—arise in many important real-world problems. These include airline scheduling, pattern recognition, circuit wiring, packing objects of various sizes and shapes into a physical space or (mathematically similarly) encoded messages into a communications channel, and a vast multitude of others (including problems in logic and number theory that really are mainly interesting only to academic mathematicians).

These are all examples of what are called combinatorial optimization problems, which typically, though not always, arise from a branch of mathematics called graph theory. We'll discuss these kinds of problems in chapter 6, but what should be clear for now is that they have the property that the number of possible solutions (e.g., the number of possible tours in the TSP) grows explosively as the number N of input variables (the number of cities in the TSP) increases. Finding the best solution as N gets large may or may not be possible within a reasonable time, and one often has to be satisfied with finding one of many "near-optimal," or very good if not the best, solutions. Whichever kind of solution one seeks, it's clear that some clever programming is required. For both algorithmic and theoretical reasons, these kinds of problems have become of enormous interest to computer scientists.

What have spin glasses to do with all this? As it turns out, quite a lot. Investigations into spin glasses have turned up a

number of surprising features, one of which is that the problem of finding low-energy states of spin glasses is just another one of these kinds of problems. This led directly from studies of spin glasses to the creation of new algorithms for solving the TSP and other combinatorial optimization problems. Moreover, theoretical work trying to unravel the nature of spin glasses led to the development of analytical tools that turned out to apply nicely to these sorts of problems. So, even in the early days of spin glass research, it became clear that they could appeal to a far greater class of researchers than a narrow group of physicists and mathematicians.

## Spin glasses represent a gap in our understanding of the solid state.

Why is a crystalline solid (in which constituent atoms or molecules sit in an ordered, regular array) rigid? It may be surprising to learn that it wasn't until the twentieth century that we understood the answer to this question at a deep level.

Why is window glass (which does not have crystalline structure; the atoms sit in what look to be random locations) rigid? That's an even harder question, and you may be even more surprised to learn that we still can't answer that question at a deep level.

Of course, at what level you're satisfied with an explanation depends on your point of view: an answer that satisfies a chemist may not satisfy a physicist (and vice versa), and mathematicians are hard to convince of anything (so they're seldom satisfied). To be fair, at some level we've understood the nature of the solid state since the nineteenth century, when modern thermodynamics and statistical mechanics were developed by Gibbs, Boltzmann, and others. The basic idea is this. Atoms and molecules at close range attract each other, but they're never isolated from the rest of the

world; consequently, the constituent particles of a system always have a random kinetic energy that we measure as temperature. At higher temperatures, entropy (roughly speaking, disorder induced by random thermal motions) wins out, and we have a liquid or gas. At lower temperatures the attractive forces win out, and the system assumes a low-energy ordered state—a crystalline solid. Liquids and crystals are two different phases of matter, and the transition from one to the other, not surprisingly, is called a phase transition.

If you've taken introductory-level physics or chemistry courses you know all this. But there are deeper issues, which enter because there are features accompanying the ordered state that aren't so easy to explain. One of these is what Philip Anderson calls "generalized rigidity" [13]: when you push on the atoms in a crystal at one end, the force propagates in a more or less uniform manner throughout the crystal so that the entire solid moves as a single entity.

This is something we all take for granted. Why is it mysterious? Well, interatomic forces are short range and typically extend only about  $10^{-8}$  cm, whereas when you push on a solid at one end, the force you apply is transmitted in a perfectly uniform manner a billion or more times the range of the interatomic force. How does that happen? What changed from the liquid state, where the exact same forces are present? At the very least, why doesn't the solid crumple, or bend? (And for that matter, what new phenomena need to be invoked to explain crumpling and bending when they do happen?)

This phenomenon isn't unique to solids; the transmission of forces over long distances also occurs, for example, in liquid crystals. In fact, this property is widespread in a general sense: it occurs whenever there's a transition to an ordered state that possesses a symmetry (whose form may not always be obvious) that differs from the thermally disordered state. Without

6 Introduction

generalized rigidity, not only would solids not be "solid" but magnets wouldn't be magnetic, supercurrents wouldn't flow in superconductors, and we wouldn't be here to observe all this. All these effects have similar underlying causes, but a deep understanding based on a small set of unifying principles didn't arise until after World War II.

At this point those of you with physics or chemistry backgrounds might feel some impatience, and protest that the answer really isn't all that complicated. If all atoms place themselves at the same distance from their nearest neighbors—that is, form a crystal—then they've created a very low energy state. Deforming this state would require a large input of energy, as anyone who's ever tried to bend, tear, or deform a solid knows. This answer is perfectly correct, and is fine as far as it goes. But it's unsatisfying at several levels. For one thing, as we'll see momentarily, it fails as an explanation of why glass—which is not a crystal—is rigid. Nor does it explain the sharp discontinuity in rigidity behavior at the liquid—crystal phase transition. A few thousandths of a degree above the transition, there's no rigidity; just below, there is. Wouldn't a gradual change in rigidity as temperature is lowered make more sense? But that's not what happens.

So there's much that this simple answer leaves unexplained, and many interesting phenomena that it can't by itself predict. Additional—and deeper—principles and concepts are needed.

Generalized rigidity is one of many examples falling within the category of "emergent behavior": when you have a system of many interacting "agents"—whether they're physical particles exerting mutual forces, or interacting species in an ecosystem, or buyers and sellers in the stock market—new kinds of behavior arise that for the most part are not predictable or manifest at the level of the individual. In the case we just discussed, something new happens when atoms rearrange to form a crystal; the ability to transmit forces over large distances is not present in the

fundamental physical interactions—in this case, the interatomic forces—that ultimately give rise to this effect. Rigidity must somehow arise from the collective properties of *all* the particles and forces: what we call long-range order (long range, that is, on the scale of the fundamental interatomic force) and broken symmetry (more on that later).

The idea of emergence is probably the most common underlying thread in complexity science, but as this example shows, emergence is not confined to complex systems. (At least the authors have never heard of table salt referred to as a complex system.)

But back to glasses. The problem here is that as far as we know, there is no phase transition (which in physics has a very specific meaning) from liquid to glass, no obvious broken symmetry, and no obvious long-range order (though a number of speculative candidates for these last two have been proposed). A glass is a liquid that just gets more and more viscous and sluggish as it's cooled, until eventually it stops flowing on human timescales. (By the way, that old nugget about windows in thousand-year-old European cathedrals being thicker at the bottom than at the top as a result of glassy flow over a thousand-year period isn't so. If you see a window with this feature, it had some other, more prosaic cause. Flow in window glass at room temperature would take place on timescales much longer than the age of the universe. Glass really is rigid.)

So why is glass rigid? As of this writing, there are lots of theories and suggestions, but none that is universally accepted. The problem is that a glass is a type of disordered system—the atoms in a glass sit at random locations. But much of our current understanding of condensed matter systems—crystalline solids, ferromagnets, liquid crystals, superconductors, and so on—applies to ordered systems with well-understood symmetries that enable profound mathematical simplifications and physical insights. So it's not only our ideas on rigidity (about which we won't have much more to say) that glasses challenge.

8 Introduction

They challenge equally our understanding of many less familiar but equally fundamental properties of the condensed state. We'll encounter many of these as we go along.

An important clarification: when we talk about disorder in glasses, we're not talking about the kind you see in liquids or gases, where at any moment atoms are also at random locations. In those higher-temperature systems, the disorder arises from thermal agitation, and the atoms (or whatever individual units constitute the system) are rapidly flitting about and changing places. That enables us to do some statistical averaging, which in turn allows us to understand the system mathematically and physically. Glasses, on the other hand, are stuck, or "quenched," in a low-temperature disordered state, and so we can't apply the same set of mathematical and physical tools that we can apply to the liquid or gaseous state. And similarly, because of the lack of any kind of obvious ordering, we can't apply the same set of tools that we utilized to understand the crystalline solid state.

Spin glasses are also systems with this sort of "quenched disorder," but here the disorder is magnetic rather than structural. We'll explain this in more detail in chapter 4, but for now it's sufficient to note that spin glasses might provide a better starting point from which to develop a theory of disordered systems than ordinary glasses. That, and the fact that there's a gaping hole in our understanding of the condensed state owing to our lack of a deep understanding of systems with quenched disorder, is the reason why spin glasses have attracted so much interest among physicists and mathematicians.

## Spin glasses display features that are widespread in complex systems.

So far we've indicated why mathematicians, physicists, chemists, computer scientists, and engineers might (or should) be interested in spin glasses. But complexity studies cast a wide net,

bringing in not only workers in these fields but also biologists, economists, and other natural and social scientists of various backgrounds and interests. What about them?

This is usually the point where treatises on the subject attempt to provide a working definition of complexity. We won't attempt that here, and not only because we don't know the answer. After many years, there still is no universally accepted definition of complexity, or of how to determine whether a given system is "complex." This is not for lack of trying, and many people (including one of us) have made proposals.

But it's not our goal, and certainly not the purpose of this introduction, to concisely define complexity.<sup>3</sup> That purpose, aside from the usual one of acquainting the reader with some basic ideas and concepts, is to convince her or him that it's worth investing some time to read the rest of the book. If you're still with us, then in your case we haven't yet obviously failed, but you may still be wondering whether all this has any relevance to your own field of interest. So we'll now take a look at some of the broader impacts and applications of spin glass theory.

We'll begin the discussion by asking, what kinds of systems are generally agreed upon (even in the absence of a definition) to be complex?

A far from exhaustive list might include a wide variety of adaptive systems or processes, systems that exhibit pattern formation, scale-free systems or networks, systems with a modular or hierarchical architecture, and systems generating or incorporating large amounts of information. Of course, some of the most interesting complex systems display several or all of these features at once.

We'll briefly discuss a few examples of each. Adaptation occurs in many contexts: biological evolution, ecological networks, the immune system, learning and cognition in biological and artificial systems, adaptive computer algorithms, economic and social 10 Introduction

systems, and many more. Biological pattern formation occurs at the cellular level in morphogenesis, at the organismal level in zebra stripes and butterfly wings, and at the group level in schooling fish. Nonbiological patterns occur in cellular automata, or in physical systems far from equilibrium, such as the regularly spaced ripples that occur in sand dunes or in "cloud streets," or the oscillations that occur in certain driven chemical systems. "Scale-free" systems exhibit similar-looking structure, phenomena, or behaviors on many length- or timescales, not just one or a few. The canonical example of this is the appearance of vorticity at multiple lengthscales in turbulent fluid flow, but scale-free behavior or structure in one form or another characterizes many complex systems and networks, whether physical, biological, or social.

Almost all systems regarded as complex are out of equilibrium (defined appropriately for the system in question) and maintain themselves at the boundary between rigid ordering (as in a crystal, where not much change can occur) and chaotic flow (where, so to speak, too much change is occurring, so that no coherent ordering, evolution, or adaptation can take place). This is sometimes referred to as being at the *edge of chaos* [16, 21, 22]; these systems maintain a delicate balance so that an ordered structure can be maintained while growth, evolution, and adaptation can still occur.

Many complex systems, particularly those that are the result of some kind of evolution (biological or otherwise), are hierarchically structured. A full-blown complex structure cannot spontaneously arise all at once; a modular architecture enabling a gradual increase in complexity is needed. And finally, the above discussion implies that all complex systems possess or generate a large degree of *information*, whether in the Shannon, algorithmic, or other sense.

Perhaps one of the most important unifying features of complex systems, and one that doesn't get mentioned often enough, is that many of them surround us in the everyday world; sometimes they are even a part of us, such as our own brains or immune systems. Unlike many other systems investigated by scientists, they're typically not obscure or esoteric or known only to a small group of specialists or experts. And as a corollary, they are not idealized in any sense: they're real-world, messy systems, inspiring difficult questions that usually don't fit neatly into any one scientific category, such as biology, chemistry, or physics. They transcend disciplines, and consequently their understanding usually requires transdisciplinary collaborations and insights. All scientific problems are complicated, but only some are complex.

So, where do spin glasses fit into all of this? It's probably already apparent that spin glasses don't adapt in any usual sense of the word, nor do they form any obvious patterns. They don't evolve, change, or learn. Mostly, spin glasses just sit there.

In that case, how can they provide insights to those interested in any of the problems we just mentioned?

There are two broad classes of answer to this question. One class involves observed spin glass behaviors in the laboratory that are reminiscent of some of the features discussed above and that remain poorly understood theoretically. The other involves theoretical constructs that may in the end have little to do with real spin glasses in the laboratory (though they may—as we'll discuss in chapter 7, this remains a topic of controversy) but that nevertheless are very suggestive of general features of complexity. In the first case, we have experiments in search of a theory; in the second, theory in search of experiments. Both may have more relevance to complexity studies than to each other.

12 Introduction

One of the few things that everyone agrees on is that spin glasses are systems with both quenched disorder and frustration. We've already discussed disorder, which in one form or another is common in complexity—it's hard to imagine a complex system that is perfectly regular in any simple sense. Frustration refers to the presence of numerous constraints that conflict with each other so that not all can be simultaneously satisfied. This is clearly something that should be a universal feature of complex systems, but it was in the study of spin glasses that the idea first crystallized, was put on a mathematical footing, and developed.

Disorder and frustration often go together, but they refer to distinct concepts, and neither implies the other. In many cases—even that of structural glasses—it's not so easy to derive crisp mathematical formulations of these properties, as they apply to the system at hand. In spin glasses, this can be done readily, and so they provide a well-defined mathematical laboratory for the exploration of these concepts and their possible implications and consequences.

But it wasn't just disorder and frustration that made spin glasses so useful. They also exhibited a number of other features that many complex systems display. Moreover, in spin glasses these features arise naturally and spontaneously from a minimalist starting point; they don't have to be inserted "by hand." Such features include the presence of many near-optimal solutions, which we've already seen figures prominently in combinatorial optimization problems. In the case of spin glasses, these "solutions" refer to low-lying (in energy) metastable (or possibly thermodynamic) states. They include the generation of information (in the Shannon sense) in the selection of particular outcomes when a spin glass is cooled or an external magnetic field is removed. They include a novel and exotic hierarchical ordering of states that spontaneously emerges in at least one nonphysical

(but important) model of spin glasses. And finally, spin glasses inspired the development of new mathematical techniques, which may be applicable to other kinds of complex systems, to describe and perhaps explain all this.

Consequently, starting in the early 1980s, spin glass concepts, ideas, and mathematical tools were applied to problems in neural networks, combinatorial optimization, biological evolution, protein dynamics and folding, and other topics current in biology, computer science, mathematics and applied mathematics, and the social sciences. Some applications were reasonably successful, others less so. We'll meet some of them in chapter 6.

On the experimental side, spin glasses show some very peculiar and interesting nonequilibrium behaviors. Of these, two that are potentially most relevant for other complex systems are, first, the presence of a wide range of intrinsic relaxational or equilibrational timescales, and second, the observation of memory effects: a spin glass is able to "remember" certain features of its past history in a rather remarkable way.

Many of these properties (and others that we'll encounter as we go along) are widespread throughout complex systems from many fields. What makes the spin glass so special is that these properties all seem to arise, in one way or another, from a very simple-looking energy function that can be written down in one line. It is deeply surprising that this should be so, and we have yet to understand what general complexity principles, if any, can be learned from this. But at the very least, the emergence of all these properties, and the mathematical techniques that arose to describe them, have proved useful in a wide range of studies that go far beyond the original problem of understanding an obscure class of magnetically disordered systems.

So it may well be the case that in learning something about spin glasses, you might uncover some new insights and tools to 14 Introduction

help you better understand your own system of interest. And very possibly, even if you don't, it might still be entertaining to learn how so many new, fundamental, and useful concepts can arise from studying such an initially boring-looking and unpromising system—which is where we started the discussion.

#### 1

### ORDER, SYMMETRY, AND THE ORGANIZATION OF MATTER

Quarks, strings, and black holes receive much of the attention that the popular press devotes to physics, and for good reason: they're exciting, exotic, and almost mystical in their appeal. They're also comfortably removed from the everyday world around us. We may be ultimately composed of vibrating stringlike excitations, and black holes may govern the history and future of the universe we live in, but for most of us, their impact on our daily lives is nil.

Does that mean that these subjects are of no real value, aside from providing intellectual entertainment for some (and for a very few, the source of their monthly paycheck)? At the moment, perhaps it does; but it's good to remember that a couple of hundred years ago, electricity also had no relevance to people's everyday lives. In the early nineteenth century, experiments on electricity and its counterpart, magnetism, were the provenance of a very small number of scientists working in isolated laboratories. Today, we automatically expect a lighted room when we flip

a switch, and many of us have a meltdown when our computer hangs for more than a few seconds.

In the industrialized world, almost everyone's daily life—in fact, our physical well-being—depends completely on the thenesoteric discoveries of scientists in the nineteenth century who worked on electricity, magnetism, light, and the thermodynamic properties of solids, liquids, and gases, and those in the twentieth century who brought us quantum mechanics and with it a modern understanding of atoms and molecules, and how they organize themselves on a macroscopic scale: what has come to be called *condensed matter physics*. The last seeks to investigate the collective behavior of many interacting units (usually but not necessarily atoms), and as a practical matter includes the study of solids, magnets, superconductors, liquid crystals, and other ordered media.

Our point isn't so much that we all owe a debt of gratitude to our scientific forebears (though we do) but rather that the distinction between "practical," "applied," and "relevant," on the one hand, and "pure" and "esoteric" on the other isn't as sharp as our prejudices might lead us to believe. As was the case with electricity and magnetism, that distinction may break down over time.

But that's not all that quarks and strings might have in common with the semiconductors from which your computer is made. Common intellectual threads permeate our understanding of why solids behave the way they do, and why electrons, quarks, gluons, the Higgs particle, and the rest of the menagerie of particles and fields that make up the fabric of our world behave the way they do.

That is, just as the distinction between practical and pure is more fuzzy than we tend to think, so is the distinction between the exciting-sounding world of particles and strings and the comparatively boring, staid one of solids. There is a shared intellectual framework that underlies our physical and mathematical understanding of all of these. And at the heart of that framework lie the unifying ideas of *order* and *symmetry*.

In this short primer, we won't have space to devote to the intellectual convergence of particle and condensed matter physics, which represents one of the great triumphs of late twentieth-century physics. It's sufficient that this convergence already illustrates that fundamental ideas can cut across and unify disciplines that on the surface address very dissimilar systems. This will be a central theme for us also, as we explore the connection between spin glasses and complexity science. It also raises an important question of what we mean—or perhaps should mean—by "fundamental."

But we'll return to all that later. Now that we (hopefully) have your attention, we'll turn to a brief discussion of the basic concepts of order and symmetry, which form not only the beginning of our story but also much of its heart.

#### 1.1 The Symmetry of Physical Laws

In its everyday use, "symmetry" has many meanings. The bilateral symmetry displayed by many organisms (including us), the stripes on a zebra, the spiral placement of petals in certain flowers, the repetitive arrangement of atoms in a crystal—we perceive all of these as highly symmetric arrangements.

In everyday usage, the idea of symmetry strongly overlaps the notion of patterns. And most of us find these patterns deeply pleasing, for they provide not only the visual enjoyment of observing natural or artifically constructed patterns in space but also the auditory pleasures of music, which consists of complex patterns of audible frequencies in time. Science aside, the perception and appreciation of pattern and symmetry in

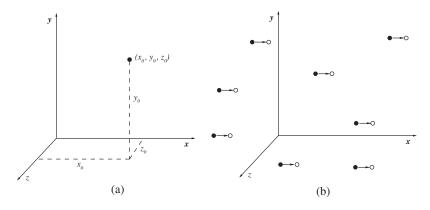


Figure 1.1. (a) Particle at  $(x(t), y(t), z(t)) = (x_0, y_0, z_0)$ . (b) A system of particles undergoing spatial translation to the right by one unit. If a given particle was originally at the position (x(t), y(t), z(t)) (filled circle), its new position (at the same instant t) is at (x(t) + 1, y(t), z(t)) (open circle).

space and time are woven into some of our most enjoyable experiences.

In physics also, symmetry brings deep intellectual pleasure to those who study it. But here its meaning is different: the notion of symmetry concerns how the laws of nature change—or don't change—when they undergo some sort of theoretically applied *transformation*. By transformation, we mean the (imaginary) alteration of the state of every particle in some prespecified, mathematically definable way. As an example, consider a collection of particles zipping to and fro. At any time t, each particle is at a position given by the coordinates (x(t), y(t), z(t)) relative to some arbitrary but fixed coordinate system, as in figure 1.1(a).

One example of a physical transformation is every particle instantanously moving (as an imaginary exercise, remember) to the right by, say, 1 cm. This is called a *space translation*, and an example is shown in figure 1.1(b). Another possible

transformation is the mirror inversion of a system; this is called a *reflection*. Yet another is particles rotating each through some fixed angle about an internal axis, with their relative positions unchanged (this makes sense only if the particles are not point-like but instead have internal structure, like footballs or tennis rackets).

These are all examples of *spatial transformations*, and of course there are many others.<sup>2</sup>

Transformations in time are also possible. One of the most important is simply a *time reversal*. If you're watching a movie of water molecules zipping around, you can effect a time reversal by simply running the movie backward and observing the results.<sup>3</sup>

There are many other types of transformations as well: particles suddenly changing their velocities<sup>4</sup>; wavefront locations changing in a system of waves, known as a *phase transformation*<sup>5</sup>; and more. But we hope that by now you get the point.

What interests physicists is what happens to the laws of nature—Newton's equations of motion, Maxwell's equations of electric and magnetic fields, Schrödinger's equation of wave mechanics, and other equations that govern the behavior of matter and energy—when certain transformations are applied. Do the laws (i.e., equations) remain unchanged? If so, they are said to be *symmetric* under those transformations, and that usually carries deep implications.

Here's a simple example to illustrate this idea. Consider a system of particles obeying Newton's second law of motion,  $\mathbf{F} = m\mathbf{a}$ . Here  $\mathbf{F}$  is some outside force applied to a particle of mass m, which consequently undergoes an acceleration  $\mathbf{a}$ . We're usually interested in cases where the force  $\mathbf{F}$  depends only on position, such as the gravitational or electrostatic force, each of which famously varies as the inverse square of the mutual distance between two particles. In the example considered here we'll assume that the only forces on each

particle arise from its interactions with the other particles in the system.

Now suppose we apply a uniform space translation, that is,  $\mathbf{r} \to \mathbf{r} + \mathbf{c}$ , where  $\mathbf{c}$  is an arbitrary, constant vector. This notation means that at any given instant, we take every particle and shift its position by the same amount  $\mathbf{c}$ . How does this affect Newton's second law of motion? Does it change? To answer this, we have to examine the effect of the transformation on each of the terms in the second law.

The simplest term to consider is the mass: certainly, changing the position of a particle leaves its mass unaffected. We next look at the force felt by each particle. A uniform space translation clearly leaves this unchanged as well, because only the *relative* distance between particles matters, and every particle is shifted by exactly the same amount.

That leaves the acceleration. To see what happens to it, let  $\mathbf{r}'$  be the new position of a particle, originally at position  $\mathbf{r}$ , after the transformation,<sup>8</sup> that is,  $\mathbf{r}' = \mathbf{r} + \mathbf{c}$ . The acceleration  $\mathbf{a}$  is formally the second derivative of the instantaneous position  $\mathbf{r}(t)$  of a particle, where t is the time:  $\mathbf{a} = d^2\mathbf{r}/dt^2$ . Therefore, after the transformation the new acceleration  $\mathbf{a}'$  is

$$\mathbf{a}' = \frac{d^2 \mathbf{r}'}{dt^2} = \frac{d^2 (\mathbf{r} + \mathbf{c})}{dt^2} = \frac{d^2 \mathbf{r}}{dt^2} + \frac{d^2 \mathbf{c}}{dt^2} = \frac{d^2 \mathbf{r}}{dt^2} = \mathbf{a}, \quad (1.1)$$

so  $\mathbf{a}' = \mathbf{a}$ . In deriving equation (1.1) we used the fact that  $\mathbf{c}$  is constant, so its derivatives are zero.

Because all of the terms in Newton's equations of motion remain unchanged under a uniform space translation, we say that Newton's laws (at least when the forces depend only on the relative particle positions) are *symmetric*—or more properly, *invariant*—under uniform space translations. It's easy to show (convince yourself) that the same is true for time translations

 $t \rightarrow t + t_0$ , where  $t_0$  is a constant; that is, we shift time backward or forward by some fixed amount.

Perhaps more surprising is that Newton's laws are invariant under *time reversal*, in which we run time backward. Mathematically, this corresponds to the transformation  $t \to -t$ ; that is, wherever you see the variable t in an equation, replace it by -t. Since the forces depend only on positions, they're independent of t, so they can't be affected. Mass as usual is unaffected, and acceleration is likewise unchanged. To see the latter, let u = -t, and use the chain rule twice. You'll find  $d\mathbf{r}/du = -d\mathbf{r}/dt$ , but  $d^2\mathbf{r}/du^2 = d^2\mathbf{r}/dt^2$ . The first of these says that under time reversal, velocities are reversed ( $\mathbf{v}' = -\mathbf{v}$ )—exactly what you'd expect if you ran a film backward. But *accelerations* are unaffected:  $\mathbf{a}' = \mathbf{a}$ .

This means that you can't tell the difference if a film of a swarm of stars moving under their mutual gravitational attraction is run forward or backward, and similarly for a movie of water molecules moving under their mutual intermolecular forces. This may surprise you, because our experience is that everyday life is emphatically *not* symmetric under time reversal: we remember the past but not the future; we age but don't grow younger; an egg dropped on the floor splatters, but the reverse never happens. In every real-life situation we can think of, we certainly *can* tell the difference if a film of those activities is run forward or backward.

Nevertheless, most laws of physics really are time reversal invariant. Why this stunning dichotomy exists between everyday experience and the laws of physics that such experiences must obey is an interesting and deep question, but one that's tangential to our main focus here. So let's return to discussing the implications of these symmetries.

One of the most famous is a theorem from 1918 due to Emmy Noether, showing that symmetries of physical laws in space and time imply corresponding *conservation laws*. The symmetries in her theorem refer to those within an underlying mathematical construction that gives rise to equations of motion, <sup>10</sup> but never mind the details: the consequences of Noether's theorem are profound. For example, if a system's equations of motion are unchanged under space translations, then its linear momentum is conserved: the sum of the momenta of all the objects in the system remains constant in time. Similarly, symmetry under uniform rotations corresponds to conservation of angular momentum, and symmetry under time translations (meaning the underlying equations don't change in time) leads to conservation of energy.

This can be extended to the entire universe: if space is *homogeneous*, meaning that the physical laws of the universe are the same here as at its other end, then the total momentum of all particles in the universe is conserved. If space is *isotropic*, meaning that the laws of physics are the same regardless of the direction you look, then the total angular momentum of the universe is conserved. Finally, if the laws of physics don't change in time (which we're not absolutely sure about), then the total energy of the universe is conserved.

Symmetry and its consequences are among the great organizing principles of physics research in the modern era. Most fundamental laws, whether in particle physics or in condensed matter physics, possess numerous symmetries of many types, and we have learned a great deal by uncovering these symmetries and studying their consequences.

It might then come as something of a surprise that one of the most striking features of the world we live in is that it is manifestly *not* very symmetric, although the underlying laws governing it are. The lack of time-reversal symmetry in the everyday macroscopic world is one prominent example, but there are many other interesting cases, to which we now turn.

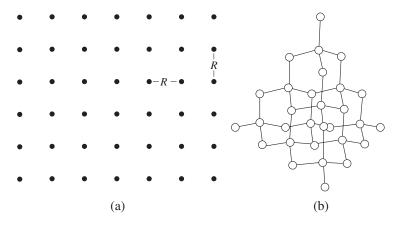


Figure 1.2. (a) A sketch of the arrangement of atoms in a simplified twodimensional crystal, a square lattice with lattice constant *R*. (b) A balland-stick model of the three-dimensional arrangement of carbon atoms in diamond. From [26], p. 6.

### 1.2 The Hamiltonian

No physical system better represents popular notions of order and symmetry than the crystal. To a physicist, the term encompasses more than solids such as gems, minerals, or grains of table salt, all of which manifestly display a crystalline structure. A sheet of aluminum or chunk of copper also fits the bill. In fact, almost all simple, conventional solids are crystals, in which the building blocks (usually atoms or molecules) repeat in a perfectly regular array. The shortest distance in a given direction in which the lattice repeats itself is called the *lattice constant*. A sketch of a simple two-dimensional crystal with lattice constant *R* is given in figure 1.2(a).

Of course, figure 1.2(a) is only a cartoon. Real crystals tend to have much more complicated structures, often with different lattice constants in each of the three spatial directions; an example is the three-dimensional arrangement of carbon atoms in diamond, shown in figure 1.2(b). But the underlying idea is the same: the atomic structure of a crystal possesses an ordered regularity that extends over very long distances. <sup>11</sup> This property, reasonably enough, is called *long-range order*.

What will probably surprise those new to this is that the physicist regards the crystal as having *less* symmetry than the corresponding liquid or gas. This is opposite to our usual usage of the term "symmetry," which tends to conflate it with notions of order. In physics, the two are intimately related, but not interchangeable: to the physicist, the crystal is *more* ordered but *less* symmetric than the liquid. Let's see why this is.

The starting point for analyzing the thermodynamic behavior of a many-body condensed matter system is the energy function that governs the arrangements of its elementary constituents. For specificity, let's choose for our example a crystal made of argon. The "units" that make up the crystal are the individual argon atoms, each with the same mass m. Let's suppose that the crystal comprises N such atoms, where N is typically on the order of  $10^{23}$  or  $10^{24}$ . The ith atom is completely characterized by its momentum  $\mathbf{p}_i$  and its position  $\mathbf{r}_i$ .  $^{12,13}$  We'll denote by  $\mathcal{H}_i$  the energy of the ith atom; it includes both its kinetic energy  $p_i^2/2m$  and potential energy. The latter arises from the forces acting on atom i from all other atoms in the crystal.  $^{14}$ 

In the case of argon these interatomic forces are called van der Waals forces, which arise from fluctuating electric fields stemming from internal atomic motions, but we don't really need this level of specificity. It's enough to realize that almost always, the forces between atoms in a crystal depend only on their *relative* positions, and so we can generally write the potential energy of atom i arising from the force exerted on it by atom j (and vice versa) as  $V(|\mathbf{r}_i - \mathbf{r}_j|)$ . That is, the mutual force between two atoms, and consequently the resulting potential energy,

depends only on their mutual distance. Equally important, it's almost always true that the range of the interatomic forces, and therefore the potentials as well, is roughly  $10^{-8}$  cm. If the distance  $(|\mathbf{r}_i - \mathbf{r}_j|)$  is of this order or smaller, then the potential energy term describing the effect of atom i on atom j is appreciable; otherwise, it's effectively zero.

Putting everything together, the total energy of atom i at any moment is

$$\mathcal{H}_i = \mathbf{p}_i^2 / 2m + \sum_{j=1, j \neq i}^N V(|\mathbf{r}_i - \mathbf{r}_j|)$$
 (1.2)

because the potential energy of atom i arises from its interactions with all of the other atoms in the crystal (even though most of the terms in the sum are very close to zero). The total energy  $\mathcal H$  of the crystal is then simply the sum of the individual atomic energies (counting the potential energy contribution from each pair of atoms only once):

$$\mathcal{H} = \sum_{1 \le i \le N} \mathbf{p}_i^2 / 2m + \sum_{1 \le i < j \le N} V(|\mathbf{r}_i - \mathbf{r}_j|). \tag{1.3}$$

This is called the *Hamiltonian* of the crystal, named after William Rowan Hamilton, who in the early nineteenth century helped place classical mechanics on a deeper mathematical footing.

Notice that the Hamiltonian depends on a very large number of variables, known as *degrees of freedom*. In three dimensions, the state of a given atom at any moment is described by six independent variables: the components of its momentum in the x, y, and z directions and the x, y, and z components of its position vector. With N atoms, this amounts in total to 6N independent variables, or degrees of freedom. So what equation (1.3) does is tell us the total energy of the system—a single number—given the 6N independent degrees of freedom listing the momenta and positions of all N atoms at any time.

(Of course, to compute the energy, we ultimately need a specific form for the potential energy V, which depends on the type of atom.)

Although we've called equation (1.3) the crystal Hamiltonian, there is nothing apparent in it that refers to any crystal. The Hamiltonian (1.3) simply describes the total energy of a collection of N argon atoms, moving and interacting via mutual interatomic forces. The same Hamiltonian describes gaseous argon, liquid argon, and solid argon equally well. So how or where does it contain information describing any of these states of matter? This is a crucial question, and we'll return to it in section 1.5, but first we need to explore further the properties of the Hamiltonian.

# 1.3 Broken Symmetry

Now let's examine the symmetries of the crystal Hamiltonian. The most important is translational symmetry. Under the transformation  $\mathbf{r}_i \to \mathbf{r}'_i = \mathbf{r}_i + \mathbf{c}$ , where  $\mathbf{c}$  is an arbitrary constant vector, the Hamiltonian remains unchanged: the momentum  $\mathbf{p}_i = m d\mathbf{r}_i/dt$  is unaffected, as is any potential of the form  $V(|\mathbf{r}_i - \mathbf{r}_j|)$ .

Now we can answer the question of why the crystal is regarded as having *less* symmetry than the liquid or gas. Refer back to figure 1.2(a), and ask yourself which spatial symmetries it possesses. That is, under which spatial transformations does the crystal structure "return to itself," meaning that the final picture is indistinguishable from the initial picture, as in figure 1.3(a)?

Figure 1.3(a) shows a uniform translation to the right by the lattice constant R. Of course, there are other obvious translational symmetries: if you shift every atom to the right, left, up, down, or some combination thereof by an integer multiple of R, the

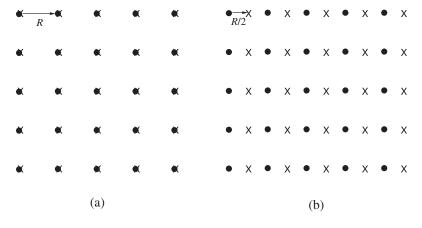


Figure 1.3. Translations of a crystal that (a) do and (b) do not return to the initial state. Initial positions of the atoms are indicated by filled circles and final positions by  $\times$ 's. In (a), all atoms are shifted rightward by one lattice constant, R (an infinite crystal is assumed). In (b), they're shifted to the right by *half* a lattice constant, R/2.

resulting picture is again unchanged. So, under many (infinitely many, in fact) uniform translations the crystal returns to itself—but certainly not under all, as seen in figure 1.3(b).

Needless to say, we're not just restricted to translations. You may have noticed that if you *rotate* the crystal in figure 1.2(a) about any atom by a multiple of 90°, it again returns to itself. So the crystal also displays certain *rotational symmetries*.

Notice that we're making a couple of assumptions here. The first is that all of the atoms are indistinguishable, so there's no difference in the picture if we rotate or translate, because we're not labeling the atoms individually. This is not just a fictional convenience; owing to their quantum mechanical nature, atoms of the same element really *are* indistinguishable. The second assumption—and this is more of a stretch—is that the crystal is of infinite extent: to have perfect periodicity, the crystal must

extend forever in every direction. In a real crystal, the periodicity is disrupted at its boundaries. But in light of the size of a crystal compared to that of an individual atom, this approximation describes well the "bulk" properties of the solid. In other words, what happens deep in the interior is largely unaffected by what goes on at the surface.

So it's safe to say that the crystal possesses a large degree of symmetry. Given that, why are we saying that it actually has *less* symmetry than the liquid or gas?

To see why, take a look again at Hamiltonian (1.3) in the limit  $N \to \infty$ , corresponding to an infinite system. Notice that the Hamiltonian is unchanged—or, in physics parlance, is invariant—under rotations of *any* angle about *any* axis. The rotational symmetry of the crystal, on the other hand, is much more limited: it is invariant only through 90° rotations (or multiples thereof) about certain axes, namely, those going right through the atoms or at certain other carefully selected points. Clearly, the set of rotational symmetries of the crystal is much smaller than that of the underlying Hamiltonian describing the physics of interacting argon atoms.

The same is true for translational symmetries: the Hamiltonian is invariant under translations of any amount in any direction, whereas the crystal is invariant only under translations that are integer multiples of the lattice constant along a few special directions (see figure 1.3).

What about the liquid and gas? Figure 1.4 shows three snapshots, at different moments, of the atomic positions (indicated by filled circles) and momenta (indicated by arrows) in the liquid or gaseous state. <sup>16</sup>

Any one of these snapshots clearly isn't invariant under rotations or translations. But there's an important difference from the crystal: no matter what the starting configuration, in the liquid or gaseous state each atom can eventually assume pretty

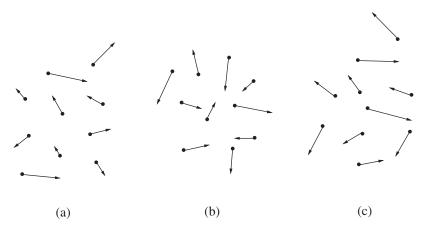


Figure 1.4. Three snapshots of atoms in the liquid state. Arrows indicate the momenta of individual atoms.

much *any* position and momentum.<sup>17</sup> On the other hand, in an undisturbed crystal the atoms are pretty much stuck where they are.

For this reason, we consider the liquid and gaseous phases as retaining the full symmetry of the Hamiltonian: no particular set of points in space has been singled out as special. The crystal, on the other hand, has "chosen" such a set, thereby greatly restricting its possible symmetric transformations; and so we say that in the crystalline phase, the symmetry of the Hamiltonian is "broken."

Why does this matter? Remember that the Hamiltonian arises from the underlying physical laws determining interatomic forces and consequently overall system energies. So the low-temperature phase—that is, the crystal—does *not* reflect the full symmetry of the underlying laws that gave rise to it. This sounds as though it should have consequences. And, of course, it does.

Before we get into that discussion, though, we need to address one more issue. Why do we call it "broken" symmetry as opposed

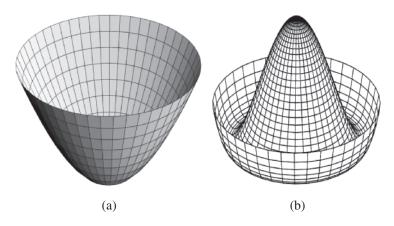


Figure 1.5. Surface at (a) high temperature and (b) low temperature. As the temperature lowers, the surface deforms continuously from (a) to (b). From http://en.wikipedia.org/wiki/Paraboloid and http://en.wikipedia.org/wiki/Spontaneous\_symmetry\_breaking.

to, say, "lesser" or "reduced" symmetry? The former connotes a more or less active process, while the latter invokes passivity. The answer is that the crystal has an infinite number of ways in which it can "break" the symmetry, but ultimately it must choose just one (we ask the reader to indulge us in our anthropomorphic imagery).

Figure 1.5 may help to illustrate this. Imagine the entire system represented as a marble sitting on a surface whose shape changes with temperature. <sup>18</sup> At high temperatures the surface is a paraboloid of revolution, and the marble has no choice but to sit smack in the center. This is a perfectly symmetric situation. But as the temperature lowers, the bottom of the paraboloid progressively flattens, and at some point the surface changes its qualitative features, taking on the shape shown in figure 1.5(b), with the center now rising. Now the center, which had previously been a stable point (in the sense that if you moved the marble

slightly away, it would roll right back), becomes unstable:—a slight push in any direction and the marble rolls away. It is a priori equally likely to roll in any direction—it can end up at any one of an infinite number of points along the circle representing the energy minimum—but it *must* end up at one.

How does the marble choose the point at which it ultimately lies? We generally can't say. It's sitting right in the center as the temperature lowers, and just when the shape of the surface changes, whatever chance breeze happens to come along—a random fluctuation here, a stray field there—pushes it slightly away from the center, after which it continues to roll downhill. The information as to where the marble ends up is not contained in the surface, which at all temperatures is perfectly rotationally symmetric about the center. If we repeat the process many times on identical systems, we'll end up with a different result—that is, a different final resting place for the marble—every time.

In every case, the final state does not reflect the symmetry of the surface; it is the system itself that in some way or another "chooses" the final state. For this reason the full name for this phenomenon is *spontaneously broken symmetry* (though in usage the "spontaneously" is often dropped).<sup>19</sup>

Back to the crystal. Figure 1.6 shows, relative to a fixed coordinate axis, three equally likely outcomes when the crystal is formed. Once again, an infinite number of final possibilities exists; in each, the crystal is shifted slightly.<sup>20</sup> But any crystal can choose only one.

#### 1.4 The Order Parameter

We noted earlier that broken symmetry carries significant consequences. One of these is the emergence of *Goldstone modes*: collective large-scale, low-energy "excited" configurations above

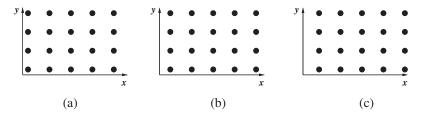


Figure 1.6. Crystal with three outcomes relative to a fixed coordinate axis.

the lowest-energy state.<sup>21</sup> Sound waves in crystals are an example of a Goldstone mode; the Higgs particle, which has attracted much media attention in recent years, is another.<sup>22</sup>

But a discussion of these collective excitations would take us too far afield of our central objective, namely, to introduce the basic ideas needed to understand spin glasses (and no more). There is, though, another consequence of broken symmetry that *will* be important, and that is the emergence of a new thermodynamic variable needed to describe a system's broken symmetry. This new variable is called the *order parameter*.<sup>23</sup>

Thermodynamic variables describe with a handful of numbers the internal collective state of a huge number of particles (typically of order  $10^{23}$  or more). You may be familiar with some of these (if not, no cause for worry; we'll define what's needed as it arises). They include the total internal energy, entropy, and volume of a system. If the system also possesses electric or magnetic properties, then the thermodynamic variables include other quantities that we'll meet up with shortly, such as the total internal magnetization.

These variables depend in turn on other, *external* parameters that affect the state of the system and that an experimenter can usually directly control—the temperature the system is held at, the pressure it's subjected to, an external magnetic field (if present), and so on.

The order parameter is a new thermodynamic variable that also describes the internal state of the system—in this case, how it broke its symmetry. Consider again the marble in figure 1.5. The order parameter here would tell us where the marble's final resting state is with respect to the coordinate axes. At high temperatures, it's always at the origin. Once the potential changes shape, though, taking on the form shown in figure 1.5(b), we need *two* numbers to describe the marble's position. One is its distance from the origin, which depends on the temperature,<sup>24</sup> but at *fixed* temperature will be the same for any possible outcome. This is sometimes referred to as the *amplitude* of the order parameter. But we also want to know *where* on the circle the marble rests, that is, *how* it broke the rotational symmetry. This can be described as an angle—called the *phase*<sup>25</sup> of the order parameter—that the marble makes with the *x*-axis.

Even though this is an artificial example, it contains the basic features of the simpler sorts of order parameters. It is zero in the high-temperature, or symmetric, state, but at low temperature takes on a nonzero value, consisting of (at least) an amplitude and phase that specify the exact nature of the broken symmetry.

To summarize, order parameters contain information about the nature and extent of symmetry breaking. By "nature," we mean the kinds of symmetries (translational, rotational, or other) found in the system Hamiltonian and that are broken in the low-temperature phase. The amplitude of the order parameter contains information about the *extent* of symmetry breaking, while its phase enables us to pinpoint *how* the symmetry is broken. For example, consider a crystal at rest with respect to a fixed coordinate system. The order parameter here tells us not only the magnitudes and directions of the lattice constants but also where the atom nearest the origin lies, and (looking ahead) in a ferromagnet, it tells us both the magnitude of the macroscopic magnetization and in which direction it's pointing.

So what is the order parameter for a crystal? This is a little difficult to describe in words, and we'll have to be satisfied with a rough description. We need to find a function that is zero in the liquid or gaseous phases and whose amplitude and phase allow us to reconstruct any crystal structure—including exactly where in space the atoms are all sitting. This can be accomplished by constructing a "density wave" function, by which we mean the following. The average density in a given volume of space is the amount of matter contained within, divided by the volume. In a crystal, <sup>26</sup> the density is periodic in all three spatial directions: large in the region where the atoms are sitting and small in the spaces between. So the order parameter should be a function (or set of functions) whose amplitude is nonzero when all the atoms (not just a few) are periodically located with just the right spacing along the right directions, and zero otherwise. In a liquid, there might be some short-range correlations in atomic positions, but none over long distances, and the correlations are even shorter range for a gas. So the order parameter for both of these will be zero.

To construct such a function requires a branch of mathematics called Fourier analysis, but we're not going to go into that level of detail; we just want to give a flavor of what's going on. In fact, we won't need the order parameter of a crystal in what follows; it serves only as an illustration. As we'll see in chapter 3, the order parameters that we *will* need, namely, those for ferromagnets, are much easier to visualize and describe mathematically. For now, it's enough to note that the crystal order parameter, true to its name, describes its long-range order. It contains the information needed to specify the probability of finding an atom anywhere in the crystal.

Although we've focused on the crystal so far, much of what we've learned will carry over more generally to other condensed matter systems. The lowest energy state of a system is commonly called its *ground state*. In the case of a crystal—and, as we'll see, in many other systems—the ground state breaks the symmetry inherent in the Hamiltonian.

### 1.5 Phases of Matter

Up to this point we've focused on the Hamiltonian, which allows us to compute the energy of any configuration of the microscopic constituents of a condensed matter system. More than that, the Hamiltonian encapsulates the essential physics of the system and contains all the information we need to describe the system's macroscopic behavior.

But something is clearly missing. We noted earlier that the crystal Hamiltonian describes equally well the solid, liquid, and gaseous phases of a particular substance. So how do we know the material's behavior when it is subjected to different external environments—that is, different temperatures, pressures, magnetic fields, and so on? The job of extracting that information belongs to *statistical mechanics*, the branch of physics that provides a microscopic basis for thermodynamics.

Of course, we're not going to try to sneak in a course in statistical mechanics in this primer. In fact, we're going to try to boil the entire subject down to a single main idea. <sup>27</sup> To keep things simple, let's hold all possible variables fixed: the number of particles in the system (which we assume is very large, at least of order  $10^{23}$ ), the volume, and so on. The only external parameter we'll vary is the temperature, which we'll denote as T. <sup>28</sup>

The main idea of statistical mechanics is that the temperature acts as a sort of "probability tuner" to tell us which configurations<sup>29</sup> of the degrees of freedom are likely to be present. Specifically, the relative probability of a configuration with energy E appearing at a given moment is proportional,

up to an overall normalizing constant, to  $e^{-E/k_BT}$ , where  $k_B$  is Boltzmann's constant.<sup>30,31</sup> The factor  $e^{-E/k_BT}$  is called the *Boltzmann factor*, and a distribution of configurations appearing with relative probabilities given by their respective Boltzmann factors is called a *Boltzmann distribution*. A system whose configurations are Boltzmann distributed is in thermodynamic equilibrium (and otherwise it's not).

The upshot is that at any fixed temperature, configurations with energy significantly larger than the temperature are strongly suppressed; that is, the probability of any of these configurations appearing at that temperature is extremely low. All other configurations, that is, those with energies roughly equal to or smaller than the fixed temperature, will likely appear. <sup>32</sup>

Of course, there's a lot more to the story. One of the most important observations is that the higher the energy, the larger the number of *different* configurations that have roughly that energy. Referring back to figure 1.4, the three configurations shown are different, but all of them—and an astronomical number of others, when N is large—share more or less the same energy. The number of configurations within the same narrow energy range provides a measure of what is known as the *entropy* of the system: entropy is large when there are many configurations with roughly the same energy. In general, the higher the energy, the higher the entropy, and consequently—given the role of the Boltzmann factor just described—the higher the temperature, the higher the entropy of the resulting *thermodynamic state*. <sup>33</sup>

When the temperature is high enough, there are many configurations that are allowed and that are microscopically distinct, but statistically look the same to us (just as there are many ways for a room to be messy or a collection of books to be out of order, but we generally don't care about the details). Every second the system passes through trillions (chosen from a much, much larger number) of such available states, flitting unimaginably quickly

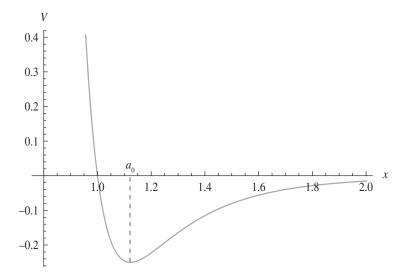


Figure 1.7. Sketch of the van der Waals potential energy between two interacting argon atoms as a function of their mutual distance. Units are arbitrary, but the scale of the energy is order  $10^{-21}$  J and the scale of the distance is  $10^{-8}$  cm.

from one to the other. This is what we see as the liquid—or at even higher temperatures, the gaseous—state. Both are thermally disordered states with high entropy.

As the temperature is lowered, however, these disordered configurations become "frozen out": the system is increasingly unlikely to assume any of them. At low enough temperature, the only configurations likely to appear are the relatively few with very low energy. What do they look like?

Well, let's take a look at the interatomic van der Waals potential that governs the interactions of argon atoms. As a function of x, the separation between two argon atoms, it looks roughly like the sketch in figure 1.7.

We see that two atoms have the lowest mutual energy when they are a certain distance (denoted by  $a_0$ ) apart; typically,  $a_0$  is

roughly of order  $10^{-8}$  cm. If the atoms are closer than  $a_0$ , there's a repulsive force that pushes them apart;<sup>34</sup> farther away, and an attractive force pulls them together. Notice also that the attractive force falls quickly to zero as the atoms separate beyond a few  $a_0$ . Extrapolating to a large system, we conclude that its *overall lowest energy* occurs when *all* of the atoms are a distance  $a_0$  from their nearest neighbors—which is, of course, the structure of the crystal.<sup>35</sup>

But that can't be all there is to it. After all, isn't this configuration also allowed when the temperature is high? Yes, it is; only configurations with energy much larger than the temperature are suppressed. But there are, relatively speaking, very few ways of arranging the atoms to form a crystal, while there is an astronomical number of ways of arranging the atoms in any old disordered configuration. So even if a crystal-like arrangement of atoms does momentarily appear—very unlikely, because there are so few of them out of an astronomical number of arrangements to choose from—all that would happen is that the system would flit rapidly back to a disordered configuration. The very low entropy of the crystalline configuration effectively removes it from playing any role in determining the system's nature at high temperature.<sup>36</sup> The upshot is that the crystalline state plays a substantial role only at sufficiently low temperatures, when higher-energy disordered configurations are frozen out.

The preceding discussion can be summarized by noting that the phase of a system is determined by an interplay between energy and entropy, with temperature acting as a "tuner" controlling (through the Boltzmann factor) the relative influence of each. This idea is neatly and succinctly captured by a new thermodynamic variable called the *free energy*. There are several different formulations of free energy, depending on the system environment; the simplest<sup>37</sup> applies to situations where temperature, volume, and number of particles are all held fixed.

The free energy is then defined to be (total internal energy) minus (temperature)×(entropy), and is minimized by a system in equilibrium.<sup>38</sup> One can then see that at low temperature, the tendency to minimize energy dominates, leading to the system preferring an ordered configuration—in the case of argon, the crystal. At higher temperature, the tendency to maximize entropy dominates, and the system prefers a disordered configuration: the liquid at intermediate temperatures, and the gas at high temperatures.

#### 1.6 Phase Transitions

Starting with a Hamiltonian and adding the tools of statistical mechanics, we've arrived at a deeper picture underlying the everyday experience that an ordinary material is a gas at high temperatures, a liquid at intermediate temperatures, and a crystal at low temperatures. But what characterizes the *transition* from one state of matter, or *phase*, to another?

Here things become interesting indeed. It turns out there's no continuous transition from liquid to crystal: the change in phase is sharp, occurring suddenly and discontinuously. At one atmosphere of pressure, water is liquid ever so slightly above 0°C and becomes ice just below. We referred in the introduction to this discontinuous change as a *phase transition*, and research into the properties of phase transitions—which come in several different flavors—constitutes an entire field of study in itself.

Phase transitions represent a *physical* as opposed to a chemical change of a macroscopic system: the abrupt, wholesale rearrangement of its (chemically unchanged) microscopic constituents. Phase transitions can occur without any breaking of symmetry, as in the transition from liquid to gas. But we'll mostly be interested in those that *are* accompanied by a change in symmetry.



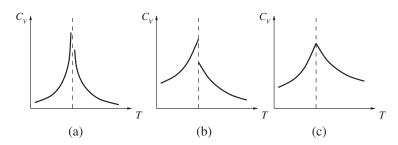


Figure 1.8. Three discontinuous changes in the specific heat. In (a), the specific heat diverges both above and below the transition. In (b), the specific heat remains finite everywhere but is discontinuous at the transition. In (c), the specific heat is continuous everywhere, but its first derivative is discontinuous at the transition.

Here the order parameter abruptly changes at the transition; in the symmetric (i.e., high-temperature) phase its magnitude is zero, but it becomes nonzero in the nonsymmetric (low-temperature) phase. In some systems a nonzero order parameter appears discontinuously, jumping from zero to a nonzero value as the transition temperature is crossed; in others, it rises continuously from zero (but with a discontinuous derivative).

The presence of sharp changes is a general feature of phase transitions. It applies to most or all (depending on specifics) of the thermodynamic variables—or their derivatives—that describe the material in question. One such variable relevant to a wide variety of systems is  $C_V$ , the specific heat at constant volume. This measures the heat flow into or out of a system when the temperature is changed by a small amount; mathematically, it can be written  $C_V = T(\partial S/\partial T)$ , where S is entropy and it is understood that the volume and number of particles in the system are held fixed. Depending on the material and the nature of the transition, there are several ways in which  $C_V$  can change abruptly. Three of these are shown in figure 1.8.

These and similar discontinuities or singularities in thermodynamic functions, under carefully controlled conditions (to be discussed further in section 2.1), usually present a clear experimental signal of a phase transition. The sharp delineation of a system comprising many degrees of freedom into separate and well-defined phases, each with its own distinct thermodynamic properties, is central to our understanding of condensed matter physics.

# 1.7 Summary: The Unity of Condensed Matter Physics

By the early 1970s, condensed matter physics had arrived at a unified synthesis of ideas, providing a deep and extensive basis for understanding the organization of matter. The engine behind the spectacular advances of the mid- to late twentieth century was the powerful set of insights and tools provided by the simultaneous exploitation of quantum mechanics and statistical mechanics. Further developments led to the profound idea of symmetry breaking and its consequences: the nature of the ground state and its collective excitations, and the identification of a new thermodynamic variable called the order parameter. Add to this the sharp delineation of the organization of matter into separate phases and the suddenness of the transitions between these phases as temperature (or pressure, or magnetic field, or other external control parameter) is varied, and you've arrived at a deep and comprehensive framework for understanding the nature of the condensed state.<sup>39</sup>

Combined, these concepts provide a powerful means of analyzing and understanding a wide variety of condensed matter systems, including crystals, different types of magnets, superconductors and superfluids, liquid crystals, ferroelectrics, and many others. When a new type of condensed matter system appears—and they do continue to appear, most recently the well-publicized high-temperature superconductors and the less well-publicized but also important two-dimensional electron liquids—these concepts provide a basis to begin theoretical analysis and supply a guide to experimental investigations.

This is, of course, a far cry from asserting that the problems posed by the discovery of a new type of condensed matter system are thereby easy to solve. Life is never so simple. 40 But they do provide a widely applicable framework of ideas to organize our thinking.

There remains an important caveat: the unified basis of understanding that we've laid out applies to *ordered* media, in which symmetries and regularities provide powerful physical insights and mathematical simplifications. When such regularities are *not* present, as happens in glasses and spin glasses, we're at somewhat of a loss as to how to proceed. We'll take up these issues in the next chapter.

#### GLASSES AND QUENCHED DISORDER

When we discussed in section 1.6 the discontinuous behavior of thermodynamic functions at a phase transition, we referred (somewhat obliquely) to "carefully controlled conditions." To proceed to the next part of our story, we need to explain just what we meant by this. To do so, we turn to the central notion of *thermodynamic equilibrium*.

# 2.1 Equilibrium and Nonequilibrium

The goal of thermodynamics is to obtain as economical a description as possible of a macroscopic system comprising a huge collection of interacting atomic- or subatomic-sized units. A glass of water consists of order  $10^{24}$  water molecules; how do we describe its physical state? What we *don't* need, even if it could be obtained (and it can't), is a list of the positions and momenta of all the water molecules. What would we do with such a list? And even if we had one, it would become obsolete in an instant: all

of the molecules are continually racing about and colliding, changing their positions and momenta every picosecond.

What we *can* make use of is a handful of measurable, macroscopic observables that describe the *overall* state of the water: its volume, temperature, the pressure it exerts on the walls of its container, and a few other variables. Roughly speaking, we say that the system is in thermodynamic equilibrium when this handful of variables—or, more accurately, a properly chosen subset—completely characterizes the system.

This requires further explanation. Note first that—again in contrast to everyday usage—"equilibrium" is not synonymous with "quiescence." Certainly, you wouldn't think of a nonquiescent system—a rushing river, say, or an exploding star—as being in equilibrium, and you'd be right. But many quiescent objects are decidedly *not* in equilibrium. A prominent example is glass, which in a real sense is *more* quiescent than a glass of water. Although both look quiet on human-sized length- and timescales, the story is very different at the microscopic level: in water, as already noted, the molecules are constantly zipping about, while in glass they mostly stay put.

If quiescence is not by itself sufficient, how do we determine whether a given system is in thermodynamic equilibrium? This is not always so easy, and as we'll see later, this difficulty has been a major stumbling block in interpreting both laboratory and numerical experiments on spin glasses. But there are certain requirements that a system in equilibrium must satisfy, making it easy in at least some cases to determine that an object is *not* in equilibrium. Stasis on the macroscopic level is one: if temperature or pressure is changing in time, the system is not in equilibrium. <sup>1</sup> Another prerequisite, in isolated simple systems at least, is homogeneity: temperature, pressure, and other attributes should be uniform throughout the sample. If they're not, the system is generally not in equilibrium.

Most important, the macroscopic properties of a system in equilibrium are independent of its history. The state of a system should be describable solely by a handful of numbers specifying volume, temperature, and so on. Further, these (unchanging) numbers should arise from the internal (rapidly changing) microscopic configurations of the system and nothing else: not how the system was initially prepared, not how it got to its present state, and not how long it's been *in* its present state.

It is this crucial feature of history independence that a glass lacks. The characterization and behavior of a piece of glass strongly depend on its past; consequently, glass is out of equilibrium.

#### 2.2 The Glass Transition

For perspective, let's compare the processes by which a crystal and glass respectively are formed, each starting from the hightemperature liquid state. A crystal results from cooling a liquid sufficiently slowly that the system remains in equilibrium throughout the cooling process. To make this more precise, imagine starting with a liquid in equilibrium at a fixed temperature. Now lower the temperature by a very small amount. This will temporarily throw the liquid out of equilibrium, but it possesses an intrinsic temperature-dependent relaxational timescale, which measures how long the liquid takes to make the necessary internal rearrangements so that it returns to an equilibrium state at the new, lower temperature. By continually dropping the temperature by small amounts and then waiting until the liquid "relaxes" to equilibrium at the new temperature, one can approximate a socalled quasi-static process. This is an idealized process in which the temperature is lowered sufficiently slowly that the liquid remains in equilibrium throughout.

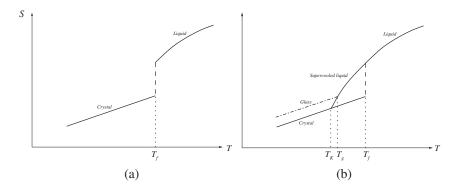


Figure 2.1. (a) Entropy (S) versus temperature (T) at fixed pressure during a quasi-static process, showing the crystallization transition at a unique  $T_f$ . (b) Entropy versus temperature during a non-quasi-static process, in which crystallization is avoided. The glass transition is shown as  $T_g$ , which depends on (among other things) the cooling rate. The Kauzmann temperature, described in the text, is indicated as  $T_K$ .

If the liquid is cooled quasi-statically, then, at some sharp and well-defined freezing temperature  $T_f$ , a phase transition occurs and the liquid crystallizes. This is illustrated in figure 2.1(a), in which the sudden and discontinuous jump in entropy S signals the transition.<sup>2</sup> At fixed pressure, the freezing temperature  $T_f$  is uniquely determined, regardless of the starting temperature, the initial state of the liquid, or the specifics of the cooling process. All that matters is that the process was quasi-static, so that the system (mostly) remained in equilibrium throughout the cooling process.

What happens when the process is not quasi-static, that is, when the cooling is done sufficiently quickly?<sup>3</sup> Now the crystalline state can often be bypassed altogether, with the system remaining in the liquid state *below*  $T_f$ , as shown in figure 2.1(b). This state is known as a *supercooled* liquid.

But this can't go on forever. As noted by Walter Kauzmann in 1948 [30], the entropy of the liquid drops more rapidly than that of the corresponding crystal, and eventually, if nothing

intervened to stop it, the two entropies would meet at a nonzero temperature. And if you kept going, the liquid entropy would fall *below* that of the crystal. The idea of a disordered liquid achieving a lower entropy than an ordered crystal is perplexing—entropy, after all, is a measure of disorder—and the phenomenon has come to be called the *Kauzmann paradox*.

But this is an extrapolation; in real systems, this entropy crossing never happens. If you manage to keep the system in the supercooled liquid state—not always easy, because often a small disturbance will cause explosively rapid crystallization—you'll find that as the temperature continues to lower, the liquid responds increasingly sluggishly as its flow becomes more viscous. This is because its relaxational and equilibration timescales are increasing rapidly.<sup>4</sup>

What this means is that it's getting increasingly harder to keep the liquid in equilibrium.<sup>5</sup> Finally, at some temperature  $T_g$ , called the *glass transition* temperature, the liquid has become so sluggish that long-range molecular motion stops, the system falls out of equilibrium, and you have a glass.

Now, the glass transition is *not* a phase transition. The glass transition temperature  $T_g$  is not uniquely determined by the system and its environment but varies depending on the cooling rate and other variable factors. It is therefore history dependent. Moreover, no thermodynamic functions display discontinuities at  $T_g$ , though some, like the specific heat, often change rapidly in its vicinity. All that appears to be happening is that the growing relaxational timescale of the liquid, which determines the time it takes to equilibrate when the temperature changes by a small amount, has crossed the human observational timescale, throwing the system out of equilibrium. This is a dynamical, not a thermodynamic, phenomenon.

All of this implies that the glass is not a phase of matter separate from the liquid. Put crudely, it's just an "arrested" liquid,



Figure 2.2. Sketch of the quenched atomic (or molecular) positions in a glass.

one in which translational molecular motion has stopped. If you were to look at the molecular positions in the glass, they would look something like that shown in figure 2.2, as if you took a snapshot of the molecules in a liquid. In particular, the ordered arrangement of the crystal in figure 1.2 is absent.

By now you've figured out that "glass" is a generic term that refers to much more than ordinary window glass. It encompasses a wide variety of solidlike materials in which crystallization has been bypassed and the molecules are frozen—or "quenched"—into a disordered configuration. We've already mentioned that glass remains an enigma to physicists: the Kauzmann paradox, the rapid increase in viscosity and relaxational timescales in the supercooled liquid state, the emergence of rigidity without order or broken symmetry, and a number of other puzzles have kept the nature of glasses a central mystery in condensed matter physics.

#### 2.3 Localization

Before moving on to other topics, we should avoid leaving the impression that research into the glassy state has been bereft of important breakthroughs, including some that might serve as fundamental and unifying concepts for disordered systems more generally. Perhaps the most important of these is *localization*, introduced and analyzed by Philip Anderson in 1958 [35]. This concerns the behavior of electrons in disordered media—namely, glasses—and as such belongs to the realm of quantum mechanics rather than classical physics, which we've largely confined ourselves to until now.

It had been known since the late 1920s, almost as soon as modern quantum theory was formulated, that an electron in a solid behaves like a wave with very special properties that reflect the periodicity of the crystal. This result, which holds for any periodic arrangement of atoms or ions and thus is completely general, was discovered by Felix Bloch, and the resulting electronic state is known as a *Bloch wave* [36]. One of the key features of a Bloch wave is that it extends over the entire crystal. This insight is crucial to understanding why certain solids, namely metals, conduct electricity and heat so well.<sup>8</sup>

Three decades later, Anderson studied the question of what an electron wave looks like in a material where the atoms were randomly located, and discovered that (with sufficient disorder) it was *localized*; it doesn't spread through the glassy material as it would in a crystal. Because of this, electrons are not mobile in a glass in the same way they are in a crystal.

This insight was crucial to understanding many of the differences between the electronic and thermal properties of glasses, on the one hand, and crystals on the other, and remains a key concept in our understanding of disordered materials.

Localization won't play a role in what follows, although its tools and conceptual underpinnings may someday prove important in spin glass theory. But given its central role as one of the great (and few) successes in our understanding of quenched disorder in condensed matter, we would be remiss in not mentioning it.

# 3

### MAGNETIC SYSTEMS

Up to this point our discussion has centered on some basic concepts of condensed matter physics as viewed through the illustrative lenses of familiar systems: liquids, crystals, and glasses. We now turn to another important class of materials: magnetic systems, which we'll regard as materials possessing properties that can be altered or manipulated through the application of an external magnetic field.

Of course, these categories overlap: a magnet can be crystalline or glassy, solid or liquid. What's really changing is our focus on the behaviors we'd like to understand. The same piece of iron might be of interest to some investigators for its crystalline properties and to others for its magnetic ones.<sup>1</sup>

# 3.1 Spin

The origin of magnetic behavior in many materials, and certainly in the more familiar magnets, arises from an intrinsic quantum mechanical property of the electron called *spin*.<sup>2</sup> The name

implies that the electron is spinning like a top about some internal axis, but this is really a poor picture of what's going on.

For one thing, as near as we can tell the electron is a point particle with no internal structure, so it's hard to say exactly what is doing the actual spinning. To be sure, the electron does possess an intrinsic angular momentum, even when it's not orbiting anything, and this is what spin refers to. But in some respects spin doesn't act like ordinary angular momentum. We can increase or decrease the angular momentum of a top by speeding it up or slowing it down, and when it stops it has no angular momentum at all. But this is not true for the electron (and many other subatomic particles). The magnitude of its intrinsic angular momentum cannot be increased or decreased; all that can be changed is its direction. It's a perfectly fixed feature of the electron, as much a part of its internal nature as its mass or charge: it's a part of the electron wherever it goes and whatever it does.<sup>3</sup>

So spin is truly a quantum mechanical feature with no classical analog. In one respect, though, its presence does carry a consequence with a classical counterpart. In classical physics, a spinning, electrically charged ball generates a magnetic field that is indistinguishable (if you don't get too close) from that of a simple bar magnet with a north and south pole. The electron, which carries a negative charge, similarly behaves like a tiny permanent bar magnet, clearly as a consequence of its spin. Pictorially, we represent both the electron's intrinsic angular momentum and its corresponding intrinsic magnetic moment (a vector quantity indicating the strength and direction of its magnetism) by an arrow, the usual symbol of a vector quantity. And, following usual practice, we will loosely and somewhat sloppily refer to both with the single term "spin," though strictly speaking this refers to the intrinsic angular momentum only.

So, in a magnetic system, the interesting degrees of freedom are not atoms but rather the subatomic electron spins. However, in the materials we'll be interested in, the electrons—and therefore their spins—are "attached" to the atoms that constitute the material. So for the most part, the spins don't change their locations.

### 3.2 Magnetism in Solids

The study of magnetism in solids is a branch of physics all to itself. Solid state magnetism takes many forms, displays many phenomena, and can arise from diverse, often complicated, atomic-level causes. Here we'll consider only two of the most common forms of solid state magnetism: ferromagnetism and antiferromagnetism.

Ferromagnetism is the most familiar form of solid magnetism, and lies behind the behavior of both permanent magnets and the solids they attract. As the name implies, it refers to the type of magnetism found in iron, but it appears in a variety of solids composed of various elements and compounds. Examples of elemental solids displaying ferromagnetism include manganese, cobalt, nickel, gadolinium, and dysprosium. The permanent magnets you probably played with as a kid and now use to affix notes to your refrigerator are alloys containing some of these elements.

Antiferromagnetism, which we'll describe soon, is also a fairly common form of magnetic behavior. Among the elements, only chromium forms an antiferromagnetic solid. The rest are compound solids, alloys, and the occasional large organic molecule. A familiar group of antiferromagnetic solids is the metal oxides—in other words, rust.

If you're familiar with the periodic table, or at least have one handy, you'll notice that all of the aforementioned elements belong to the transition metal or rare earth groups. What their atoms all have in common are unfilled d- or f-orbital subshells. If you've forgotten your chemistry, no worries: the upshot is that in most other elements, the spins of the atomic electrons cancel each other. That is, for every electron spin pointing in one direction, there's another pointing in exactly the opposite one. In contrast, most transition metal and rare earth atoms contain "leftover" electrons in their incomplete shells, with the consequence that their spins are not canceled; hence the atom itself acts as a tiny permanent magnet. For such an atom, sitting at position  $\mathbf{x}$  in a solid, we'll refer to its atomic magnetic moment (due to the uncanceled electron spins, as just described) as  $\mathbf{m}_{\mathbf{x}}$ .

If placed in a magnetic field, denoted  $\mathbf{H}$ , the atomic magnetic moment  $\mathbf{m_x}$  can lower its energy by rotating to align with the field. <sup>5,6</sup> In physics parlance, we say simply that uncanceled spins "couple" to a magnetic field. The field  $\mathbf{H}$  experienced by a particular atomic spin can include contributions from both outside and inside the solid: outside from an external magnetic field in which an experimenter may place the entire solid and inside from the combined fields of all the other atomic magnetic moments in the solid.

Suppose now that we turn off all magnetic fields outside the solid, so that the only remaining fields are internal, arising from the spins within the solid. What happens? This depends on several things. First, the situation is far more complicated than what you would encounter with a bunch of freely suspended magnets interacting only with each other. Far from being a passive bystander, the solid plays an active role in determining how the spins interact with—that is, couple to—each other. All electron spins are identical, but how they couple to each other can vary greatly depending on the local environment in which they find themselves. This is why some solids are ferromagnets, others are antiferromagnets, and

still others display increasingly exotic forms of solid magnetic behavior.

# 3.3 The Paramagnetic Phase

Regardless of how a solid behaves magnetically at low temperatures, at high temperatures<sup>8</sup> it will behave pretty much the same as any other magnetic solid. This is because the spins can couple to lots of things within the solid besides other spins, and all of them fluctuate randomly at high temperature. Consequently, as temperature rises, a given spin is increasingly jostled, pointing in different random directions from one moment to the next.<sup>9</sup> Other spins are being knocked about also, so on top of everything else, the spin is subject to a fluctuating internal magnetic field.

At sufficiently high temperatures (and zero external magnetic field), the spins are completely disordered owing to thermal agitation, so that

$$\langle \mathbf{m_x} \rangle \equiv \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^{\tau} \mathbf{m_x}(t) dt = 0,$$
 (3.1)

where  $\langle \mathbf{m_x} \rangle$  denotes the time average of  $\mathbf{m_x}$ . At high temperatures, equation (3.1) holds for *all* of the spins, and we say that the solid is in the *paramagnetic* phase. A snapshot of the paramagnetic phase is shown in figure 3.1.<sup>10</sup>

# 3.4 Magnetization

Since we prefer to look at systems on a macroscopic scale, we need a new thermodynamic variable that provides a measure describing what *all* the spins are doing. This is most simply provided by a spatial average over the orientations of all spins. This spatial

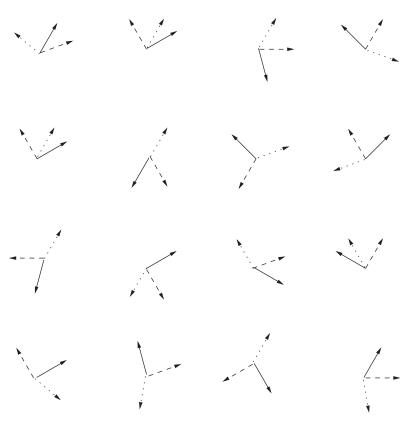


Figure 3.1. Sketch of the paramagnetic phase at three different instants of time. The arrows indicate the directions of the atomic magnetic moments for each site of the lattice. Solid arrows denote the magnetic moments at one instant of time, dashed arrows at another, and dotted arrows at a third. At a *single* site, the *time* average of the spin orientations is zero, and at each *instant*, the *spatial* average over *all* sites of the spin orientations is zero.

average is called the *magnetization*, denoted by M:

$$\mathbf{M} = (1/N) \sum_{\mathbf{x}} \langle \mathbf{m}_{\mathbf{x}} \rangle , \qquad (3.2)$$

where the sum is over all N spins in the solid. The magnetization describes the overall magnetic state of the sample, and as such, it serves for many systems as the *magnetic order parameter*. In the paramagnet,  $\mathbf{M}=0$ , so it behaves as a good order parameter should in the high-temperature phase.

# 3.5 The Ferromagnetic Phase and Magnetic Susceptibility

What happens to a paramagnetic solid in zero external field as temperature is lowered? In some solids, the coupling between nearby spins is such that their energy of interaction is lowered when they *align*. In these materials, a sharp phase transition occurs at a precisely defined temperature, denoted  $T_c$  (which depends on the material). At the atomic level, the time-averaged magnetic moment  $\langle \mathbf{m_x} \rangle$  is no longer zero; it grows as the temperature is lowered below  $T_c$ , and the thermal agitation of each spin thereby lessens. Moreover, because the interaction between nearby spins tends to align them, the magnetization  $\mathbf{M}$  is likewise nonzero below  $T_c$ .

So for  $T \geq T_c$ , the magnetization is zero, but below  $T_c$  it rises continuously from zero as the temperature continues to drop: the solid has undergone a phase transition at  $T_c$  from the paramagnetic to the ferromagnetic phase. In the ferromagnetic ground state (and ignoring quantum mechanical effects), the spins are all perfectly aligned (figure 3.2).

Unlike the liquid to crystal transition, there's no change in the appearance of the solid when it undergoes the paramagnetic to ferromagnetic phase transition. But the internal changes are nonetheless dramatic. As in other phase transitions, thermal quantities, such as specific heat, undergo discontinuities in their magnitudes or their derivatives. The solid's magnetic properties are similarly dramatically affected. To measure these, we use a



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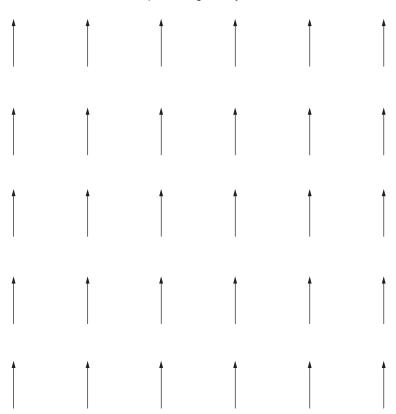


Figure 3.2. Sketch of the ferromagnetic ground state.

quantity called the *magnetic susceptibility*, denoted by  $\chi$ ; as the name implies, it measures the magnetic response of a solid to a tiny change in an externally applied field. Formally it is defined as

$$\chi = \lim_{h \to 0} \left( \frac{\partial M}{\partial h} \right)_T, \tag{3.3}$$

where h denotes the external field, and the subscript means that the measurement is taken at fixed temperature. <sup>11</sup> In reality, both the magnetization and the external field are vectors, and the

susceptibility has nine components, describing the response of the magnetization in each of the three spatial directions to the change in field in each of *its* three spatial directions. But we've kept things simple in (3.3) by referring only to scalar quantities. M refers only to the magnitude of the magnetization and b to the magnitude of the applied field; the directions of both are ignored. The susceptibility  $\chi$  diverges as T approaches  $T_c$  from above, that is, from the paramagnetic side. Below  $T_c$ ,  $\chi$  has a complicated behavior owing to a phenomenon called magnetic domains, which are important in ferromagnetism but play no role in our story.

# 3.6 The Antiferromagnetic Phase

In another class of solids, the interaction between nearby spins is such that their energy is lowest when they *antialign*, that is, point in antiparallel directions. These are the *antiferromagnets*, and their ground state is sketched in figure 3.3.<sup>12</sup>

There is again a sharp transition from the paramagnetic phase, at a temperature usually denoted  $T_N$ .<sup>13</sup> The magnetic susceptibility  $\chi$  has a kink at  $T_N$ , roughly as in figure 1.8(c) (except that there are two branches of  $\chi$  below  $T_N$ , one corresponding to the susceptibility measured in a direction parallel to the spin alignment axis and the other perpendicular to it). As in the ferromagnet,  $\langle \mathbf{m_x} \rangle \neq \mathbf{0}$  at each site  $\mathbf{x}$  for  $T < T_N$ , but unlike in the ferromagnet, M = 0 at all temperatures, as can be easily seen from figure 3.3. A slightly modified order parameter is therefore needed.<sup>14</sup>

## 3.7 Broken Symmetry and the Heisenberg Hamiltonian

We saw that in the liquid to crystal transition, translational symmetry is broken. In the transition from the paramagnet to

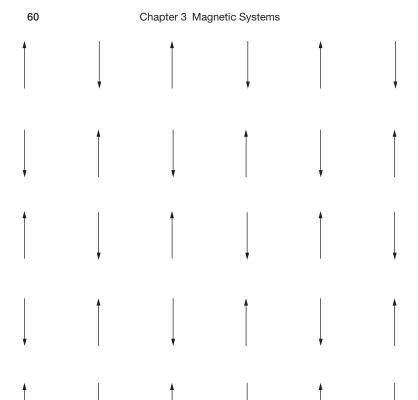


Figure 3.3. Sketch of the antiferromagnetic ground state.

either the ferromagnet or antiferromagnet, *rotational* symmetry of the spin configuration is broken. In the paramagnetic phase, every spin at any time is equally likely to point in any direction, <sup>15</sup> so the paramagnetic phase is "rotationally invariant." But in both the ferromagnetic and antiferromagnetic phases, a specific direction has been singled out, spontaneously breaking the rotational symmetry.

How do we describe all this mathematically? The starting point for many studies of magnetism in solids is a Hamiltonian originally due to Werner Heisenberg [47] and P. A. M. Dirac [48], <sup>16</sup> but these days usually called the Heisenberg Hamiltonian. In its original formulation it dealt only with quantum mechanical quantities, but a corresponding classical version has also seen a great deal of use. It is

$$\mathcal{H} = -J \sum_{\langle \mathbf{x} \mathbf{y} \rangle} \mathbf{m}_{\mathbf{x}} \cdot \mathbf{m}_{\mathbf{y}} - \mathbf{h} \cdot \sum_{\mathbf{x}} \mathbf{m}_{\mathbf{x}}. \tag{3.4}$$

Let's consider the terms one by one and see what they mean. First, the symbols used: as usual,  $\mathbf{x}$  and  $\mathbf{y}$  indicate sites in the crystal lattice. The  $\langle \mathbf{x} \mathbf{y} \rangle$  that appears under the first summation means that we don't sum over all pairs of sites but only those that are nearest neighbors. The symbol  $\mathbf{h}$  refers to a uniform external magnetic field in which the solid is immersed, and J is the coupling—that is, energy of interaction—between spins, about which we'll say more in a moment.<sup>17</sup> The individual magnetic moment  $\mathbf{m_x}^{18}$  behaves as a classical three-dimensional vector, so that the dot product  $\mathbf{m_x} \cdot \mathbf{m_y}$  is simply  $m_x m_y \cos \theta$ , where  $m_x = |\mathbf{m_x}|$  is the magnitude of  $\mathbf{m_x}$ , and  $\theta$  is the angle between  $\mathbf{m_x}$  and  $\mathbf{m_y}$ .

Now recall that physical systems like to minimize their energy—and will, if the temperature is low enough so that thermal agitation of their degrees of freedom is small. What does the Heisenberg Hamiltonian (3.4) then tell us about the low-temperature behavior of the system? The second term on the right-hand side simply says that if the solid is in an external field  $\mathbf{h}$ , each individual spin will lower its interaction energy with the field by aligning with it. But the first term is more interesting. Here J has buried within it an enormous amount of solid state physics. Its magnitude and sign vary from solid to solid.<sup>19</sup> The transition temperature, among other things, will depend on the magnitude of the "nearest-neighbor coupling" J: the larger J is, the higher  $T_c$  (or  $T_N$ ). But the sign of J is the

really interesting part: note that if J>0 (and  $\mathbf{h}=0$ ), the ground state will be the one in which all the spins are aligned, as in figure 3.2, whereas if J<0 (and  $\mathbf{h}=0$ ), the ground state will have the spins antialigned, as in figure 3.3. In other words, the Hamiltonian (3.4) describes a ferromagnet when J>0 and an antiferromagnet when J<0. Now that's economical.

Note also that, similar to what we've seen before for crystals, the Heisenberg Hamiltonian (3.4) possesses global rotational symmetry when  $\mathbf{h}=0$ : in zero external field, a magnetic system obeying (3.4) has no preferred direction. Or put another way, a global rotation of all the spins leaves the total energy invariant (just as a uniform translation of all of the atoms leaves the Hamiltonian (1.3) invariant). This rotational symmetry is present in the paramagnetic phase, in which no direction is special, but is broken in the ferromagnetic and antiferromagnetic phases, where a fixed direction is spontaneously selected.

And now we're (finally) ready to introduce spin glasses.

# 4

#### SPIN GLASSES: GENERAL FEATURES

As noted in the introduction, few things seem less likely at first glance to spark interest than the materials we now call spin glasses. Nevertheless, their rise was stunning. What one might call "sightings" of spin glasses, although they weren't realized as such at the time, appeared sporadically in the scientific literature over several decades spanning the middle part of the twentieth century (see, e.g. [49–51]). But it wasn't until the early 1970s that the condensed matter community first took serious notice of them, as a set of peculiar materials with perplexing and seemingly self-contradictory properties. Within a few years the subject had taken off as an area of intense scientific investigation, generating thousands of scientific papers by the mid-1980s.

After a series of initial experimental and theoretical successes, the questions became harder and progress slower, eventually leading many to abandon their study of spin glasses for greener scientific pastures. Still, interest in the subject remains strong, and a dedicated community of investigators continues its pursuit of the subject. As a consequence, progress, although far slower

than in the boom years of the mid-1970s to mid-1980s, continues to be made.

It is not our intention to provide anything approaching a thorough history of the subject.<sup>2</sup> The field today is broad, with threads and subthreads extending in a multitude of different directions. Given its sweep, we will confine ourselves to a relatively narrow part of the overall subject. In keeping with our<sup>3</sup> restriction of topics, we will bring in only those aspects of history relevant to the flow of the story.

# 4.1 Dilute Magnetic Alloys and the Kondo Effect

The first, though not only, class of materials that later became known as spin glasses were the dilute magnetic alloys. These are materials in which a very small concentration (at most a few percent) of a magnetic element, often iron or manganese, is substituted at random locations inside a nonmagnetic metallic host, such as one of the noble metals (copper, silver, or gold).

These alloys had been of interest to condensed matter physicists since the 1930s, when it was discovered that at extreme dilutions (usually less than a few tenths of 1% of magnetic impurity), some magnetic alloys displayed unusual and puzzling electrical conduction properties. In particular, their resistance, which in normal metals decreases and eventually flattens as the temperature is lowered, starts to rise again at a few degrees above absolute zero. This came to be known as the *Kondo effect*, after the Japanese physicist Jun Kondo, who in 1964 published a calculation that indicated how the resistance minimum arose [59]. Kondo's calculation turned out to be only the first step in unraveling this problem, whose solution had far broader implications than just explaining the peculiar conductivity properties of an obscure group of metals. It eventually opened the door to spectacular

advances not only in condensed matter physics but also in statistical mechanics and particle physics.

But that part of the story goes off in a different direction. The upshot for us is that dilute magnetic alloys quickly became interesting objects to study, and eventually investigators started wondering what would happen if you increased the concentration of magnetic impurity by a factor of 10 or more, that is, from a few tenths of 1% to a few percent.

#### 4.2 A New State of Matter?

At the extremely low concentrations of a few tenths of 1% of magnetic impurity atoms, their magnetic moments<sup>5</sup> are sufficiently far apart that their effect on one another is negligible. But one would expect that with increasing concentrations, interactions between the randomly placed, localized atomic magnetic moments should begin leading to some observable effects. And this is what typically *does* occur—beginning at quite low concentrations, often around 1%.<sup>6</sup>

In fact, by the beginning of the 1970s it was already becoming evident that some sort of magnetic ordering *should* take place in dilute magnetic alloys at impurity concentrations around a few percent.<sup>7</sup> This could already be seen in the high-temperature paramagnetic phase, where the dependence of the magnetic susceptibility on temperature deviated noticeably from what would have been seen if the magnetic moments were noninteracting.

So in some sense the condensed matter community was primed when, in 1971, Cannella, Mydosh, and Budnick [60] observed a cusp in the susceptibility of gold-iron alloys (figure 4.1). This susceptibility cusp, when measured in very small magnetic fields, has been seen many times since in a variety of materials and is one of the central experimental signatures of spin glasses.

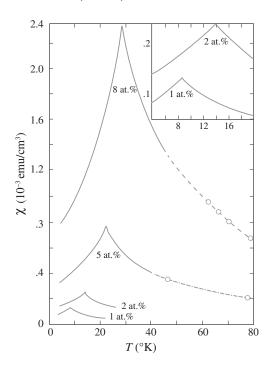


Figure 4.1. Susceptibility cusp in gold-iron alloys. The percentages indicate the concentration of iron. The circles represent isolated measurements taken at higher temperature. From [60].

It presumably signals a phase transition from a paramagnetic phase to a low-temperature phase with some sort of magnetic ordering.

In fact almost a decade earlier there had already been indications of magnetic ordering at low temperatures, at least in alloys where iron was the magnetic impurity. The details aren't important here <sup>8</sup>; what *is* of interest is that, for each impurity concentration measured, the transition temperature corresponded well to the temperature at which the susceptibility cusp occurred. So it was beginning to look very much as though some sort of phase transition was taking place.

But to what? The early experiments seemed to suggest that the low-temperature phase was antiferromagnetic (which also displays a susceptibility cusp at the transition temperature). But it soon became clear that this wasn't the case. There exists a variety of experimental probes that can provide information on what the atomic magnetic moments are doing, and measurements using these probes indicated several things. First, the spins were "frozen"; that is, unlike in the high-temperature paramagnetic phase, in which each spin flips and gyrates constantly so that its time-averaged magnetic moment is zero, at low temperatures each spin is more or less stuck in one orientation. Second, the overall magnetization was zero, ruling out a ferromagnetic phase. But third, more sensitive probes indicated there was no long-range antiferromagnetic order either: in fact, as near as could be told, the spins seemed to be frozen in *random* orientations.

This kind of behavior is already unlike our experience with more familiar magnetic materials. But at least—so far—the phase transition behavior seems fairly conventional.

But this too became murky on further probing. Recall that at a phase transition, *all* the thermodynamic functions behave singularly in one fashion or another. Surely the specific heat, one of the simplest such functions, should show a singularity as well. However, when one measures the specific heat of a typical spin glass, one sees ... absolutely nothing interesting at all. All you see is a broad, smooth, rounded maximum, which doesn't even occur at the transition temperature (defined to be where the susceptibility peak occurs). A typical such measurement is shown in figure 4.2.

We're now faced with a dilemma. Two of the central thermodynamic features of these materials exhibit contradictory behavior. The susceptibility data seem to indicate a phase transition, while the specific heat data suggest otherwise. Of course, the smooth curves shown in the figures are interpolations between

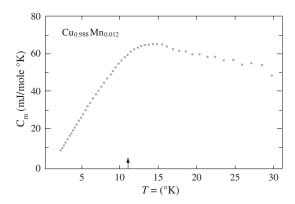


Figure 4.2. Specific heat of  $Cu_{0.988}Mn_{0.012}$ . The arrow indicates the temperature where the corresponding susceptibility cusp occurs. From [61].

data collected at a discrete set of temperatures. Perhaps if one could collect more finely spaced data near the susceptibility cusp, one might find that it becomes smoothly rounded (which in fact does happen at larger external magnetic fields). Or else, in the opposite direction, it could be that the specific heat data on finer resolution would show some small but unmistakable discontinuity.

But so far neither of these has been seen, and the low-field susceptibility cusp combined with the smooth, continuous specific heat curve has become one of the central experimental identifiers of spin glass behavior. Other identifiers include spin freezing below  $T_f$ , as we will henceforth refer to the temperature at which the static susceptibility displays a cusp. This spin freezing is coupled to a lack of any identifiable spatial magnetic order: the spins appear to point in random directions.

These four properties—a cusp in the magnetic susceptibility, a rounded maximum but no discontinuities in the specific heat, spin freezing below  $T_f$ , and an absence of spatial long-range order—together constitute the most prominent *static* features of

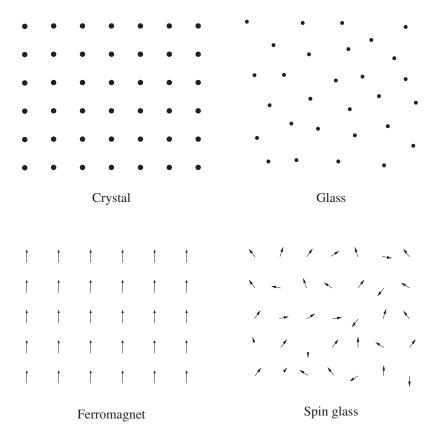


Figure 4.3. Sketches of the "ground states" of four types of condensed matter: crystals, glasses, ferromagnets, and spin glasses. Just as the atomic structure of a glass resembles a frozen "snapshot" of the liquid, the lowest-energy configurations of a spin glass resemble a frozen snapshot of a paramagnet.

materials we have come to call spin glasses. The origin of the term "spin glass" should now be clear: the last two of these properties indicate that, roughly speaking, these materials are magnetic analogs to the "ordinary" glasses described in chapter 2. Figure 4.3 should help clarify the analogy.

But this is far from the whole story. Some of the most interesting properties of spin glasses involve *dynamic*, not static, behavior, and we turn to those in the next section. For now we note that, like glasses, spin glasses possess a very broad range of relaxational and equilibrational timescales, and as a result relax and equilibrate very slowly.

This makes the issue of equilibration (section 2.1) central to the discussion. As we'll see in section 4.3, laboratory spin glasses display nonequilibrium effects, and determining whether a given sample is in thermal equilibrium can be a tricky issue, plaguing not only laboratory experiments but numerical simulations as well. Unlike with ordinary glasses, where we *know* that a sample is out of equilibrium, we're often not sure when dealing with spin glasses. And in some sense, this is really the essence of our difficulty in figuring out what the experiments are telling us.

So, returning to the topic at hand, we're faced with the following question: Is there a true thermodynamic phase transition to a low-temperature spin glass phase characterized by a new kind of magnetic ordering? Or is the spin glass just a kind of magnetic analog to an ordinary structural glass, where there is no real phase transition and the system simply falls out of equilibrium because its intrinsic relaxational timescales exceed our human observational timescales? If the latter, then the spins wouldn't really be frozen for eternity; they would just have slowed down sufficiently that they appear frozen on any timescale that we can imagine.

At first, the difference may not seem to matter much. After all, the effective motion of the spins is the same as far as we're concerned, so why bother worrying about what happens on timescales much longer than the age of the universe?

But the answer *does* matter to our understanding of the physics of these systems, and ultimately to that of quenched disordered systems in general. For it's not only the movement—or lack of it—of the spins we care about. If spin glasses turn out to be a separate thermodynamic phase with a new kind of magnetic ordering, our broader understanding of condensed matter physics will be profoundly affected. It will furthermore affect how we apply spin glass ideas to other types of problems taken from computer science, biology, and other areas—the subject of chapter 6. And it will provide deep new insights into the behavior and manipulation of not only spin glasses but possibly other disordered systems. The issue of whether the spin glass represents a new kind of thermodynamic phase will run as a central thread through our discussion as our understanding of spin glasses deepens.

As of this writing, the question remains open.

# 4.3 Nonequilibrium and Dynamical Behavior

The question of whether the spin glass is a new phase of matter concerns its equilibrium behavior. But some of the most interesting behaviors of spin glasses occur in situations that are manifestly out of equilibrium. We discussed in section 2.1 how equilibrium measurements reveal static features independent of history. Accessing these equilibrium properties requires changing external laboratory conditions such as temperature, pressure, or magnetic field in a quasi-static way, which in a practical sense means changing these quantities sufficiently slowly that the system can relax (or reequilibrate) to its new surroundings each step of the way. However, in the case of spin glasses near or below  $T_f$ , some of these relaxation times have already become so large that it's not at all clear if the system ever attained equilibrium after the temperature even got close to  $T_f$ . As discussed in the previous section, this leaves the interpretation of standard thermodynamic data—susceptibility, specific heat, and so on—open to doubt.

But situations also arise where the equilibration of the system is not in doubt—because the system is clearly *out* of equilibrium. This is the case when a property is changing with time, or when it clearly depends on how the sample was prepared (i.e., history dependence), or when the method of preparation is anything but quasi-static. An example of the latter is a "deep quench"—when the temperature rapidly plunges from high above  $T_f$  to well below.

In this section we briefly examine each of these experimental situations, all of which exhibit additional interesting spin glass behaviors. In so doing they shed light on the nature of spin glasses— while at the same time further deepening their mystery.

The first concerns what is known as "remanence" behavior of the magnetization and involves studying how spin glasses behave in moderate to strong magnetic fields (in contrast to the zero or very weak-field behavior associated with susceptibility measurements). As we've already seen (and discuss more fully in section 4.8), a spin glass in the absence of a magnetic field has zero magnetization. But it shouldn't be surprising that when placed inside a uniform magnetic field, the atomic magnetic moments will try to orient themselves along the field—as occurs in any magnetic system—resulting in a net magnetization. So far not very exciting; but what then happens after the field is removed or altered?

There are any number of ways in which this can be done, and in the spin glass they all lead to somewhat different outcomes. One approach is to cool the spin glass in a uniform magnetic field  $\mathbf{H}$  from a temperature above  $T_f$  to one well below, and then remove the field. On doing so, the spin glass at first retains a residual internal magnetization, called the *thermoremanent magnetization*. The thermoremanent magnetization decays with time, but so slowly that it remains substantial on experimental timescales.

Another procedure is to cool the spin glass below  $T_f$  in zero field, turn on a field after the cooling stops, and after some time remove the field. This gives rise to the *isothermal remanent magnetization*. In both cases the way in which the remanent magnetization changes in time depends on the history of the process, but is always exceedingly slow. Several mathematical functions have been proposed and fitted to the data over a range of timescales, including logarithmic time decay and stretched exponential  $(e^{-t^{\gamma}})$ , where t is a dimensionless time parameter and  $0 < \gamma < 1$ ). Because of the slowness of the decay, it's sometimes hard from the data to tell these different forms apart. In any case, the slow decay indicates that the process is governed by multiple relaxational timescales. <sup>11</sup>

Among the most interesting of the nonequilibrium behaviors displayed by spin glasses are *memory effects*, wherein the material seems to retain information about its past. Such effects were noticed early on in remanence experiments; for a review of these and other experiments, see [1]. Starting in the late 1980s, these effects were systematically studied in *aging* experiments [62–71].

In the simplest of these, a spin glass is cooled to a temperature below  $T_f$  in an external magnetic field, often through a deep thermal quench. The spin glass then sits at that fixed field and temperature for a certain "waiting time"  $t_w$ . After the waiting time has elapsed, the field is switched off and the decay of the thermoremanent magnetization is measured at constant temperature. Interestingly, the spin glass "remembers" the waiting time: a change in the rate of decay occurs at a time roughly  $t_w$  after the field is removed. Aging is not confined to spin glasses, but their unusual behaviors make them somewhat special.

The out-of-equilibrium behaviors of spin glasses are endlessly fascinating, and numerous theoretical approaches have been proposed to account for them. We won't delve into those

theories here but note that all share the features of a wide range of relaxational processes, leading to a broad distribution of intrinsic relaxation times; a significant amount of *metastability*, meaning that most relaxations, whether involving a small or large number of spins, can only occur after the system surmounts some energy or free energy barrier; and a consequently complicated "energy landscape," the meaning of which is discussed in section 4.9.

# 4.4 Mechanisms Underlying Spin Glass Behavior

We've seen that the magnetic, thermodynamic, and dynamical properties of certain dilute magnetic alloys display surprising, unconventional, and at times downright bizarre behavior. As it turns out, this cluster of behaviors has been seen in a variety of materials and is not at all confined to dilute magnetic alloys. In fact, many spin glasses are not metallic at all: a good number are insulators, such as europium strontium sulfide ( $Eu_xSr_{1-x}S$ ), in which the magnetic impurity europium is substituted randomly for nonmagnetic strontium, with the fraction x of europium typically a few tenths; or lithium holmium yttrium fluoride ( $LiHo_{0.167}Y_{0.833}F_4$ ), in which holmium is the magnetic ion. What do all these materials have in common?

To answer this question, we'll examine briefly the underlying solid state physics of a dilute magnetic alloy. Although the mechanism of spin glass behavior depends on the class of materials to which the spin glass belongs, there are some features shared by all classes.

Consider the isolated magnetic moment localized on a manganese impurity atom in a block of copper manganese. How can it "notice," and thereby interact with, another isolated magnetic moment localized on a distant manganese atom? Direct moment-moment coupling, such as that between two bar magnets, is too weak in this case to provide the effects seen in the lab. 14 Something must be "mediating" the interaction between the two moments. In a metal such as copper, the outermost atomic electrons leave the individual copper atoms and more or less freely roam through the metal (thus becoming *conduction electrons*). So, in an alloy like copper manganese, it might be suspected that these conduction electrons are playing some role. And that suspicion is correct.

Electron spins have two properties that are crucial to their mediation role. The first is that, as already discussed in section 3.1, electrons carry their own intrinsic magnetic moments. This means that the magnetic moments of the conduction electrons can interact with those of the localized moments on the manganese atoms, for example, through mutual spin flips as an electron passes by the manganese moment. The second is that, as quantum mechanical objects, electrons travel through metals as waves, meaning that, like all waves, electrons can exhibit diffraction and interference. For example, most people have seen bright and dark bands exhibited when light waves diffract (i.e., bend) around an obstacle or pass through a grating. These bands arise from interference: the bright parts occur where the wave amplitudes add, leading to a "stronger" wave at that location, and the dark parts reside where the wave amplitudes subtract, leading to a "weaker" wave (or no wave at all).

Something similar occurs as conduction electrons zip past and interact with the localized moment, but instead of bright and dark bands, one gets instead concentric spheres, centered on the localized manganese moment, of conduction electron spins polarized parallel and antiparallel to the localized moment. These bands of alternating conduction spin polarization are known as Ruderman-Kittel-Kasuya-Yosida (RKKY) oscillations and are illustrated in figure 4.4.

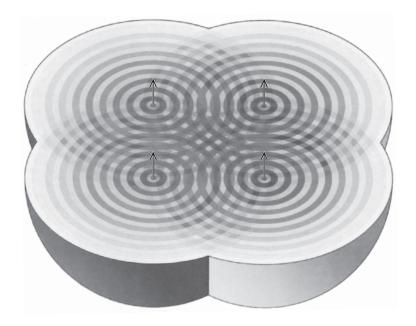


Figure 4.4. A sketch of alternating magnetic polarization of conduction electron spins due to the RKKY interaction. The spins shown represent localized manganese impurity spins. Dark concentric circles represent regions where the conduction electrons have spin polarization parallel to that of the impurity spin, while light circles represent regions with antiparallel polarization. From [11].

It is important to remember that, while the *regions* of conduction electron spin polarization are roughly static, the conduction electrons themselves are not: the physical electron is zipping along, with its spin flipping multiple times as it passes from one polarization region to another.

What follows is that, given an isolated localized magnetic moment in a metal, a second magnetic moment some distance away will find it energetically favorable to align with the first if located in a "parallel" polarization region (and consequently,

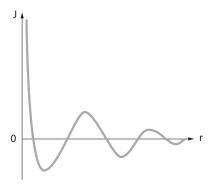


Figure 4.5. Sketch of the effective coupling function of a localized magnetic moment interacting with other localized moments via an RKKY-type exchange.

the interaction between the two will be ferromagnetic), and conversely will find it energetically favorable to antialign if located in an "antiparallel" region (the interaction is then antiferromagnetic). The effective coupling of the RKKY interaction therefore oscillates with radial distance r from the localized impurity spin and is given (for large r) by

$$J(\mathbf{r}) = J_0 \frac{\cos(2k_F r + \phi_0)}{(k_F r)^3} \,. \tag{4.1}$$

In this equation,  $k_F$ , whose inverse is roughly the size of an interatomic spacing, describes the wavelike motion of the electron and is called the Fermi wavevector, while  $\phi_0$  is simply a constant phase depending on the metal. These details are unimportant for our purposes; the two things to note are that as r changes, the effective coupling to the localized moment oscillates between ferromagnetic ( $J(\mathbf{r}) > 0$ ) and antiferromagnetic ( $J(\mathbf{r}) < 0$ )), and the interaction strength decreases (rather slowly) as r increases. The effective interaction J(r) is shown in figure 4.5.

Now, we already know that the localized moments are randomly distributed in the alloy. This means two things: first, that

two nearby localized moments in random locations have a roughly equal probability (a priori) of having either a ferromagnetic or an antiferromagnetic interaction, and second, because the magnetic moments don't migrate on experimental timescales, the interaction between any two specific moments is quenched. It is this basic property, namely, the interplay of quenched, randomly located ferromagnetic and antiferromagnetic interactions, that is believed to be primarily responsible for spin glass behavior.

The discussion so far has centered on dilute magnetic alloys, but as we already mentioned, many spin glasses belong to other classes of materials. The main point is that, in all cases, there exists a complicated arrangement of quenched, randomly placed ferromagnetic and antiferromagnetic interactions betweens pairs of spins. For example, in europium strontium sulfide, interactions between the moments on the magnetic europium atoms are (for altogether different reasons from those noted above) ferromagnetic when they're nearest-neighbors and antiferromagnetic when they're next-nearest neighbors. But, while the details differ from one class of materials to another, the essential underlying mechanism for all spin glass behavior is this interplay between quenched ferromagnetic and antiferromagnetic interactions.

#### 4.5 The Edwards-Anderson Hamiltonian

The preceding discussion may have left you with the impression that the microscopic mechanisms behind spin glass behavior in different materials are complicated and diverse. This is true, but the job of the theoretical physicist who wants to model these systems is to cut away the complicating details, which give rise to nonuniversal effects, and isolate those few features, common to all spin glasses, that lie at the heart of their behavior. This is easier said than done; skill is required to tease out the essential

from the nonessential and thereby construct a simple—or at least simple-looking—model that is mathematically well defined and that captures the essence of the spin glass.

This is precisely what Sam Edwards and Philip Anderson did in 1975 with the publication of a paper [74] that asserted that the essential mechanism underlying spin glass behavior was the presence of both ferromagnetic and antiferromagnetic interactions that were quenched randomly in place. This insight may not look like much of a leap here, especially since we already gave away the punch line in the preceding section. But we have the advantage of hindsight. At the time Edwards and Anderson wrote their paper, spin glasses were a fairly new phenomenon on the condensed matter scene and there were all sorts of proposals attempting to explain where their unusual properties came from. Edwards and Anderson proposed a Hamiltonian that is really the simplest possible one combining the essential ingredients they had identified. Forget for a moment the actual structure of copper manganese or europium strontium sulfide. Just place all the spins on a three-dimensional cubic lattice (cubes filling all of space, with a spin at each corner of every cube). Then the Edwards-Anderson (hereafter EA) Hamiltonian is

$$\mathcal{H}_{\mathcal{J}} = -\sum_{\langle x,y\rangle} J_{xy} \mathbf{m}_x \cdot \mathbf{m}_y - \mathbf{h} \cdot \sum_x \mathbf{m}_x, \tag{4.2}$$

where x, y denote sites in the cubic lattice and the notation  $\langle x, y \rangle$  means that the sum is over nearest-neighbor (i.e., adjacent) sites only;  $\mathbf{m}_x$  denotes the localized magnetic moment (or, more simply, spin), which for now we treat as a classical vector, at site x;  $J_{xy}$  is the magnetic coupling between nearest-neighbor sites x and y; and  $\mathbf{h}$  is a uniform external field (which could be zero) acting on the system.

An even simpler formulation is to treat the spins not as vectors, as in (4.2), but as simple binary variables taking on the values  $\pm 1$ 

only. Geometrically, this corresponds to each spin being allowed to point in only one of two directions, up or down. This is known as the *EA Ising model* and will play an important role in what follows. The resulting EA Hamiltonian, in which the vector  $\mathbf{m}_x$  is replaced with the scalar  $\sigma_x = \pm 1$ , and  $\mathbf{h}$  is replaced by a scalar h taking on any real value, is then

$$\mathcal{H}_{\mathcal{J}} = -\sum_{\langle x,y\rangle} J_{xy} \sigma_x \sigma_y - h \sum_x \sigma_x . \tag{4.3}$$

The basic new ingredient in (4.2) (and in (4.3)), which otherwise looks like the ordinary Heisenberg Hamiltonian (3.4), is that the couplings  $J_{xy}$  now depend on the edges  $\langle xy \rangle$ , and are chosen randomly and independently from a *probability distribution*. One choice, usually called the  $\pm J$  model in the spin glass literature, is to flip a fair coin independently for each coupling. If it comes up heads, the coupling is ferromagnetic with value +J, where J is a fixed positive constant, and if it comes up tails, it is antiferromagnetic with value -J. Another possibility is to choose the couplings from a continuous distribution  $^{15}$  such as a Gaussian  $^{16}$  with zero mean (also known as a "normal" distribution or a "bell curve," depending on one's field) and variance of order one.  $^{17}$ 

The details are unimportant for our purposes; the important thing to note for now is that the couplings are *quenched*. What this means is that, before analyzing the Hamiltonian, we first determine all the couplings by coin tossing, or whatever other method we choose; after that, they remain fixed for all time. This process leads to a particular choice, or *realization*, of the couplings, which is denoted by the symbol  $\mathcal J$  appearing in (4.2) and (4.3). Of course, there is an infinite number of coupling realizations for any probability distribution, which leads to the question, which properties depend on the specific realization and which don't? This is, in fact, an

extremely important question, to which we'll return in chapters 5 and 7.

We emphasize that the EA Hamiltonian doesn't actually look like any real spin glass. If you wanted to faithfully model a dilute magnetic alloy, for example, you would use the RKKY coupling (4.1) between all pairs of spins with the spins situated at random locations (which would then be quenched). Nevertheless, we expect the EA Hamiltonian to capture the basic physics of laboratory spin glasses. <sup>18</sup> In that sense, we hereafter refer to it as a "realistic" spin glass model.

#### 4.6 Frustration

So far we've considered systems—crystals, ferromagnets, antiferromagnets—in which the ground states are fairly easy to figure out. Moreover, as discussed in section 1.3, there are simple symmetry transformations—global translations in the case of crystals, global rotations in the cases of ferromagnets and antiferromagnets—that can transform one possible ground state into another, but we don't really consider these as distinct. We say, for example, that the ground state of the ferromagnet is one in which all the spins are aligned, and if we want to note the inherent broken symmetry, we can add, "up to a global rotation." But things are nowhere near as simple in the spin glass.

To see one reason why this is so, consider the elementary situation of four spins at the corner of a square, with three of the couplings ferromagnetic and one antiferromagnetic, as shown in figure 4.6.

We'll assume the spins are Ising, meaning (as noted earlier) that they can point only up or down. We can start by choosing the spin at the top left corner to point up, and then attempt to

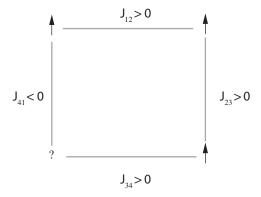


Figure 4.6. Four spins at the corners of a square, with three of the couplings ferromagnetic ( $J_{xy} > 0$ ) and one antiferromagnetic ( $J_{xy} < 0$ ). The two ferromagnetic couplings at the top and right are satisfied (meaning the spins at their endpoints are chosen so as to minimize the coupling energy, i.e., so that  $J_{xy}\sigma_x\sigma_y > 0$ ). However, no choice of the spin in the lower left corner can simultaneously satisfy both the ferromagnetic coupling at the bottom and the antiferromagnetic coupling at the left.

satisfy<sup>19</sup> the remaining couplings. But it's apparent that when we try to close the loop, we run into a conflict: there is no way that we can satisfy all the constraints imposed on the four-spin system (in this case, that means satisfying all the couplings). Such a situation is called *frustration*.<sup>20</sup> More generally, it is clear that if we take any closed cycle *C* of couplings, not all can be satisfied if the product of the couplings is negative:

$$\prod_{C} J_{xy} J_{yz} \dots J_{zx} < 0 \to \text{frustration.}$$
 (4.4)

So any real lattice in two or more dimensions will have a complicated network of interpenetrating frustrated loops. How does one then find the ground state? Which couplings should be chosen to be unsatisfied? Or are there possibly *many* ground states

not connected by any simple symmetry transformation? This is a very intriguing question, and remains one of the central unsolved problems in spin glass research. A more precise description of this problem will be given in section 7.1.

It is important to note that quenched disorder and frustration are not the same. One can have either without the other. To have disorder without frustration, one can assign quenched independent random binary variables  $\xi_x = \pm 1$  (separate from the spins  $\sigma_x$ ) to every site x in a lattice, and choose the couplings to be  $J_{xy} = \xi_x \xi_y$ . And one can have frustration without disorder: think of a pure antiferromagnet on a triangular lattice. The combination of quenched disorder and frustration makes the spin glass a very difficult problem indeed—but may also contribute to its richness of behavior and its usefulness as a model system with which to examine certain aspects of complexity.

### 4.7 Dimensionality and Phase Transitions

We now return to a question posed in section 4.2: Is there a thermodynamic phase transition to a new state of matter, that is, a spin glass phase? As of this writing, the question remains open. And at this point we need to bring up the important fact that questions of this type depend strongly on the space dimensionality of the system. Are we talking about a one-dimensional EA Ising spin glass (with the spins all on a line), or a two-dimensional EA Ising spin glass (all spins on a single plane), or a 17-dimensional one?

This may seem like another one of those questions that only a theoretical physicist can love. Certainly, three is the number of dimensions we care most about, but it's not the only one we're interested in. Lower-dimensional systems have played an important role in advances in condensed matter physics over the past few decades, displaying new phenomena unknown in ordinary three-dimensional systems and leading in a few cases to new devices.

While quasi-1D and 2D systems can be realized experimentally, what about hypothetical condensed matter systems living in dimensions higher than three? While we can't build such things, we can envision them mathematically and analyze their properties. And what we learn can very often illuminate, sometimes deeply, our understanding of ordinary three-dimensional systems. As we'll see, the greatest theoretical success in spin glasses to date has to do with the analysis and solution of a spin glass in an (effectively) *infinite* number of dimensions.

It is easy to prove theoretically that an EA spin glass in one dimension has no phase transition (but this is true for any one-dimensional system with short-range interactions only). Starting in the early 1980s, there have been numerous "experiments," conducted through large-scale numerical simulations, seeking a phase transition in higher dimensions. Based on these analyses, the current consensus is that, for the EA Ising model, there is a phase transition (at nonzero temperature) in four dimensions and higher, probably one in three dimensions as well, and none in two. But the question remains open; there has been little theoretical evidence and no mathematical proofs of any of these assertions except in infinite dimension, where we know for certain that there's a phase transition.<sup>23</sup>

The upshot is that we know for sure that there's no phase transition in one dimension and there is one in infinite dimensions. Everything in between remains conjectural. But there is numerical support for a phase transition in three dimensions and stronger numerical evidence for a transition in higher dimensions [78–80].

# 4.8 Broken Symmetry and the Edwards-Anderson Order Parameter

In addition to proposing and analyzing a simplified, general Hamiltonian for spin glasses, Edwards and Anderson asked what kind of ordering the spin glass phase, should it exist, would exhibit. (For simplicity, we take h=0 in (4.3) throughout this discussion.) Their proposal was that the spin glass is, first, disordered in *space*, so that the magnetization defined in (3.2) is zero, and similarly for other spatial order parameters that measure antiferromagnetic ordering.

They noted, however, that the spin glass should be ordered in *time*, representing the "frozenness" of the spins in the spin glass phase. That is, if you measure a spin on a particular site as pointing in a particular direction, wait an arbitrarily long time, and take another look, you'll see the spin still pointing in that direction. On the other hand, if there is no true spin glass phase, then the time correlation of spin orientation at any given site should gradually decay. This decay would be very slow, similar to the arrested, but not permanently static, flow of atoms in a glass.<sup>24</sup>

The order parameter proposed by Edwards and Anderson can be written

$$q_{EA} = \lim_{N \to \infty} (1/N) \sum_{x} \langle \sigma_x \rangle^2, \tag{4.5}$$

where, as in (3.2), N is the total number of spins in the spin glass.<sup>25</sup>

In the paramagnetic phase,  $\langle \sigma_x \rangle$  is zero at every site, so there  $q_{EA}=0$ . This reflects the spin-flip symmetry of the Hamiltonian (4.3) when h=0; a reversal of all spins leaves the energy unchanged. Edwards and Anderson proposed, however, that  $q_{EA}>0$  in the spin glass phase. For Ising spins, where each

spin can point either up or down,  $q_{EA} > 0$  implies broken spin-flip symmetry: even absent a field, a given spin is more likely to point in one direction than the other. <sup>26</sup> Of course, this is true in the ferromagnetic and antiferromagnetic and other magnetically ordered phases as well: it is the lack of any obvious spatial order, coupled with the ordering in time, that sets the spin glass apart.

But as we'll see in chapter 5, when we look at an even further simplified model of a spin glass, this may be far from the whole story. In that case, at least, things get a lot more complicated—and interesting.

# 4.9 Energy Landscapes and Metastability

We close this chapter by discussing one of the features of spin glasses that have brought them to the attention of the larger complexity community: the notion of their possessing a "rugged energy (or free energy) landscape." This is a simplified visualization of how the energy varies in the very high-dimensional space where the mutually perpendicular coordinate axes represent the orientation of each individual spin.<sup>27</sup>

The notion of an energy landscape requires a specification of spin dynamics, so let's choose a simple dynamics as follows. A spin chosen at random looks at its neighbors, and if it can lower its energy by flipping, it does so; otherwise, it stays put. This procedure is continually repeated with randomly and independently chosen spins and in so doing describes a zero-temperature, one-spin-flip dynamics. One can define a "landscape" under this dynamics: two distinct spin configurations are neighbors if they differ by a single spin, and the time evolution of the system can then be thought of as a "walk" on the landscape.

At zero temperature, the walk on the landscape is easily described: if you start with an arbitrary spin configuration and

then let the dynamics proceed, the system will simply walk downhill to the nearest energy minimum. At this point the dynamics will stop; no more spins will flip. A spin configuration that remains unchanged for all time under the dynamics is called a *fixed point* in state, or configuration, space. In principle, both the starting configuration and the specific realization of the dynamics (i.e., the specific order in which the different spins are selected for flipping) will determine the final state—that is, the fixed point the system lands in. The *basin of attraction* of a fixed point comprises all spin configurations that flow toward it under almost every<sup>28</sup> realization of the zero-temperature dynamics described above.<sup>29</sup>

Unlike the ferromagnet, in the spin glass this process will quickly stop at a relatively high-energy state. This is because the spin glass has lots of *metastability*. A one-spin-flip metastable configuration (equivalently, *local optimum*) is one in which no spin can lower its energy by the dynamics described above, but if two neighboring spins are allowed to flip simultaneously, then lower energy states are available. This concept can easily be extended to k-spin-flip metastable states, and it was proved [81] for the EA model in any dimension (including one) that, for an infinite system, there is an infinite number of k-spin-flip stable states for any finite k.

Suppose, though, that you continually increase the size of the spin clusters that are allowed to flip as a rigid unit, enabling escape from all the metastable "traps" that prevent the dynamics from reaching a true energy minimum. This leaves open the question of how many "final" states there are: two, as one would expect in the ferromagnet,<sup>30</sup> or a larger number? This is another way of restating the question of numbers of distinct ground states in a spin glass, first posed in section 4.6. A very rough way to distinguish ground states from metastable states is as follows: escaping a metastable state requires overturning a fixed number of spins, independent of the system size. On the other hand,

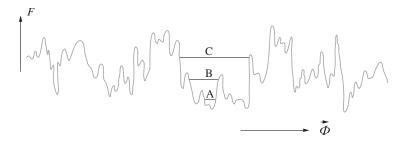


Figure 4.7. Schematic picture of a rugged energy landscape, where  $\vec{\Phi}$  is an abstract configuration coordinate. At zero temperature the system is stuck in one of many local minima; however, at positive temperature the system receives random "kicks" that can knock it out of its minimum. So at longer times or higher temperatures, more of the configuration space can be explored. From [28].

escaping a *ground* state requires overturning a number of spins that *grows* with the system size. Another way this is often stated—again, very roughly—is through the language of "energy barriers" surrounding a local optimum: typically, the larger the number of spins needed to overturn to escape a local optimum, the higher its energy barrier. In this language, metastable states are surrounded by relatively low "energy barriers," of O(1) energy, while ground states, or true global minima, are surrounded by energy barriers that grow with the size of the system<sup>31</sup> (such high energy barriers in the infinite-range version of the EA model, to be described in the next chapter, were found through numerical simulation [83]).

A pictorial representation of energy barriers is shown in figure 4.7, where relatively low barriers confine configurations to region A, those in region B are confined by higher barriers, and those in region C by still higher ones. This phenomenon (and its consequences) was dubbed "broken ergodicity" by Palmer [28].

However, a note of caution is in order: a one-dimensional picture, as in figure 4.7, can be misleading. The true configuration

space is very high-dimensional, and in high dimensions many new things can happen. In particular, a route around a mountain can often be found; one may not have to climb directly over the top [84].

The features of quenched disorder, frustration, metastability, anomalous dynamics, and rugged landscapes all contributed to the designation of spin glasses as a prototype complex system. If this were the end of the story, they would already be deserving of the interest and attention of complexity scientists.

But you undoubtedly have already guessed (tipped off at least by the presence of chapters still to come) that all this is only the beginning. And as we'll see in the next chapter, the story now takes a most unusual—and interesting—turn.

## THE INFINITE-RANGE SPIN GLASS

# 5.1 Mean Field Theory

We saw in section 1.5 how, given a Hamiltonian and using the tools of statistical mechanics, one can—in principle—completely describe a system's thermodynamic behavior at any temperature or external field. In practice, however, this is extremely difficult; if it weren't, statistical mechanics would be a closed book rather than a thriving field of active research. Very few Hamiltonians can be exactly "solved," meaning that the corresponding free energy as a function of temperature, magnetic field, and so on, can be exactly calculated. In spite of this, the thermodynamic properties of a tremendous number of physical systems have been mapped out in detail, thanks to a powerful array of mathematical tools and approximation techniques that have been developed over the years.

As one might expect, many of these tools rely on the presence of some kind of underlying order or symmetry and fail when applied to systems with quenched disorder. As discussed

in chapter 1, *all* systems are disordered at sufficiently high temperature, but that type of disorder, called *thermal disorder*, is easily dealt with. A thermally disordered material flits rapidly among many different configurations, and statistical mechanics was originally designed to handle just this kind of situation: it shows how thermodynamic properties emerge from an average over the many available states. But averaging over all allowed states no longer provides a correct thermodynamic description when quenched disorder is present: now the system is "stuck" within a small, confined subset of configurations. Moreover, the lack of any clear-cut symmetry doesn't allow for an appeal to the simplifications provided by long-range order. So it should come as no surprise that our understanding of the statistical mechanics of the EA Hamiltonian remains extremely limited.

When faced with a difficult problem like this, physicists do what anyone else would: look for a simpler but hopefully related problem. In statistical mechanics, the first recourse is usually to construct and study a so-called "mean field" version of the original Hamiltonian. This is essentially a simplified model in which every degree of freedom finds itself in the same environment as every other; in other words, local spatial fluctuations have been discarded. It is precisely these fluctuations that drive much of the interesting behavior of many phase transitions, so mean field models are often a poor guide to understanding behavior (called the critical behavior) at or near a transition. On the other hand, they're often fairly reliable at providing insights into the low-temperature properties of a system—its order parameter and broken symmetry, and the low-energy excitations that determine its thermal properties.

There are different ways in which the mean field approach can be realized, which for technical reasons turn out to be essentially equivalent. One such way is to extend the range of the interactions to infinity. This means that every spin interacts equally strongly with every other, erasing any notion of distance or geometry: everyone is effectively a nearest neighbor to everyone else. It's certainly plausible that infinite-range models and mean field models should behave similarly; what may be less obvious, but is also generally true, is that mean field theory typically becomes exact for the corresponding short-range model in the limit of infinite dimensionality [85]. In other words, the nearest-neighbor EA Hamiltonian (4.3) on an infinite-dimensional lattice is expected to behave equivalently to a model in which every spin interacts equally strongly with every other.

Technical mathematical arguments are needed to demonstrate all this, and one should be careful to note that we are not saying that mean field models, infinite-range models, and short-range models in infinite dimension are indistinguishable. The claim is that for a given system, all three should display essentially the same thermodynamic behavior, so they can be used interchangeably, but it should be remembered that the models themselves are formulated differently.<sup>2</sup>

## 5.2 The Sherrington-Kirkpatrick Hamiltonian

So, in the hope of formulating a more tractable but still useful model, David Sherrington and Scott Kirkpatrick introduced [89] an infinite-range version of the EA Hamiltonian only a few months after its first appearance. What is now called the Sherrington-Kirkpatrick (SK) Hamiltonian can be written

$$\mathcal{H}_{\mathcal{J}} = -\frac{1}{\sqrt{N}} \sum_{1 \le i < j \le N} J_{ij} \sigma_i \sigma_j - h \sum_{1 \le i \le N} \sigma_i, \qquad (5.1)$$

for a system of N spins. Note that we switched from the spin indices x, y to the labels i, j: the former denote sites on a geometric lattice, while the latter simply assign a tag to each spin—which is all we need, given that we've thrown out any geometric arrangement of the spins.

Note also the factor  $1/\sqrt{N}$ , which is new. Unlike the EA model, which has O(N) couplings for a system of N spins, the SK model has  $O(N^2)$  couplings, because each spin interacts with N-1 others. So, unless the first sum on the right-hand side of (5.1) is normalized, the model will not yield a finite energy per spin as  $N \to \infty$ .<sup>3</sup> With this normalizing factor, the couplings can be chosen from the same  $\pm J$  or Gaussian distributions, with variances of order one, as in the EA model. Finally, for simplicity we will take the coupling distribution to have mean zero and will set h=0.

If you're mainly interested in how spin glass ideas are applied to nonphysical systems, but not in the nature of spin glasses themselves, you can skip directly to section 5.7 and then on to chapter 6. But you'll miss a very interesting—and surprising—story.

## 5.3 A Problem Arises

Sherrington and Kirkpatrick went on to analyze the Hamiltonian (5.1) with Ising spins ( $\sigma_i = \pm 1$ ) and discovered two interesting things. The first is that the model has a phase transition, with critical temperature  $T_c$  determined by (and order of) the variance of the coupling distribution. It's worth jumping out of temporal sequence for a moment to point out that three years later, J.R.L. de Almeida and David Thouless [90] found that a sharp phase transition from a paramagnetic to (some sort of) spin glass phase persists even in the presence of a magnetic

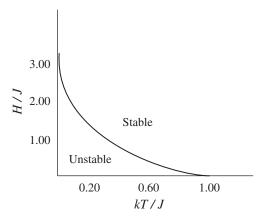


Figure 5.1. Phase diagram of the SK spin glass with Gaussian coupling distribution of mean zero and variance J in the presence of a uniform magnetic field of magnitude H. The region characterized as "stable" corresponds to the paramagnetic phase and that characterized as "unstable" to the spin glass phase. The curve separating the stable and unstable phases is the de Almeida—Thouless (AT) line. From [90].

field—something that does *not* occur for an ordinary ferromagnet. The presence of the so-called "AT line," shown in figure 5.1, is one of the distinguishing features of the infinite-range spin glass. Whether such a feature persists in short-range models remains up in the air.

Sherrington and Kirkpatrick's second finding was even more interesting: if one chooses the EA order parameter to describe the broken symmetry of the low-temperature spin glass phase, the entropy becomes negative at very low temperature. We discussed entropy in section 1.6, noting that it's related to the number of available states of a system at a given temperature. Here we need to be more precise: the entropy is defined to be proportional to the *logarithm* of the number of available states.<sup>4</sup> But the number of states can't be smaller than one, so entropy can't be negative. There must be a problem somewhere.

# 5.4 The Remedy

Sherrington and Kirkpatrick conjectured [89] (and many agreed) that the cause of the difficulty lay in the mathematical machinery used to arrive at their low-temperature solution. This was a reasonable guess: the methods used were relatively new and untested at the time, and relied on uncontrolled approximations with opaque justifications, so that even if the solution *did* make sense, no one would really understand why the procedure that led to it worked at all.

But, as it turned out, the mathematical method wasn't the culprit at all. Called the *replica method* (see [74] and references therein), it required imagining many identical but independent copies, or *replicas*, of the system; computing a thermodynamic average over them all; and then taking the number of replicas to zero. It turns out that this bizarre recipe—actually quite inspired, though mysterious—can in principle handle the difficulties posed by quenched disorder.

Over the next few years, it gradually became clear that the problem lay not in the replica procedure itself but rather in the supposition that the low-temperature broken symmetry in the SK model can be characterized solely by the EA order parameter (4.5). The story then took a turn in an even more bizarre direction: it was postulated that the symmetry that is broken is that between the replicas themselves [90].

What does that mean?

Well, just as rotational symmetry means that the Hamiltonian treats all directions equivalently, and broken rotational symmetry means that the broken-symmetric phase singles out a particular direction as special, "replica symmetry" means that the Hamiltonian treats all replicas equivalently, while broken replica symmetry means that the spin glass phase distinguishes among replicas. Insofar as the replicas were introduced as a useful

mathematical fiction, not to mention that their number is taken to zero at the end of the calculation, this all may be a little difficult to swallow.

But it gets even better. Noting *that* the replica symmetry is broken does not tell one *how* it is broken: there are many possible ways of breaking replica symmetry. And once the correct prescription is found, it should have a clear, plausible, and testable physical interpretation. It took several years to find, but what is now regarded to be the correct formulation of replica symmetry breaking for the SK model was introduced by Giorgio Parisi in 1979 [91]. From here on, when we refer to replica symmetry breaking (hereafter denoted RSB), we mean that invoked by Parisi to solve the SK Hamiltonian (5.1).

If you find the mathematics described above murky, you're not alone. So we'll now leave all that behind. The rest of this section is devoted to describing the novel features of RSB and explaining what they mean physically for the nature of the spin glass phase in the SK model. In particular (with one more dive into the murky depths), we'll attempt to transcribe into simple language and ideas the following concise (if at first glance impenetrable) quote [92] on the essence of RSB:

the Gibbs equilibrium measure decomposes into a mixture of many pure states. This phenomenon was first studied in detail in the mean field theory of spin glasses, where it received the name of replica symmetry breaking. But it can be defined and easily extended to other systems, by considering an order parameter function, the overlap distribution function. This function measures the probability that two configurations of the system, picked up independently with the Gibbs measure, lie at a given distance from each other. Replica symmetry breaking is made manifest when this function is nontrivial.

To begin, we need to introduce the notion of *thermodynamic* state.

## 5.5 Thermodynamic States

Thermodynamic states (also known as Gibbs states, Gibbs equilibrium measures, or simply Gibbs measures), very briefly introduced in section 1.5, characterize the macroscopic nature of many-body systems. They can be defined for systems with either finite or infinite numbers of degrees of freedom; for now, we'll gloss over the issues and complications that arise in distinguishing between the two, and will return for a more careful treatment in section 7.2. Here we state things as succinetly as possible: *a thermodynamic state of a spin system is simply a probability measure on its spin configurations*.

In other words, if we assign a label to every spin, then a given thermodynamic state specifies the probability of occurrence of each configuration of any finite *subset* of spins; specifically, at any moment it tells you the probability that spin 1 is up, spin 18 is down, and spin 486 is down, and similarly for any other finite collection of spins you care to inquire about.<sup>5</sup>

We've already encountered several examples of thermodynamic states: for a collection of atoms, the gas, liquid, and crystal are all examples of thermodynamic states. For an Ising ferromagnet, the paramagnetic phase (M=0), the positively magnetized ferromagnetic phase (M>0), and the negatively magnetized ferromagnetic phase (M<0) are similarly examples of thermodynamic states. Each of these implies different probabilities from the others for finding spins in given orientations: in the positively magnetized phase, a randomly chosen spin is much more likely to be found up rather than down; in the negatively magnetized phase, the opposite is true; and in the

paramagnetic phase, any spin is as likely to be pointing up as down.<sup>6</sup>

All of the thermodynamic states mentioned above are special: they are *pure states*, which will be defined in section 7.2. Here it's sufficient to note that pure states are the "physical" thermodynamic states—that is, any real material in thermal equilibrium is always in a pure thermodynamic state. Mathematically, however, we're not confined to pure states alone, and it will often be advantageous to look at their linear combinations, called *mixed states*. Again, we'll return to all this in section 7.2; for now, we don't need to worry about these distinctions, and we'll just talk about thermodynamic states in general.

# 5.6 The Meaning of Replica Symmetry Breaking

We can now return to Parisi's solution. First, we recall that the EA order parameter measures the degree of broken spin-flip symmetry. If it alone specified the symmetry breaking in the spin glass phase, then at low temperature the spin glass would be in one of two thermodynamic states, each of which is a global flip of the other. That is, if in one state (at some fixed temperature *T*) spin 7 has probability 3/4 of pointing up and spin 18 has probability 1/5 of pointing down, then in the globally flipped state spin 7 has probability 3/4 of pointing down and spin 18 has probability 1/5 of pointing up, and so on. Although both states have zero magnetization, they are clearly different.

The reason why the SK low-temperature solution failed is that, while spin-flip symmetry is indeed broken in the SK model at low temperatures (which means that all spin glass states come in globally spin-reversed pairs, like the two above), *this alone is not sufficient* to characterize the low-temperature phase. Rather than a single order parameter, there are *infinitely many*. In other

words, for an infinite system there is not a single globally spinreversed pair of spin glass thermodynamic states, but infinitely many such pairs of states. All have zero magnetization, but all also have different probabilities of finding any set of spins in a given configuration. Moreover, none of the different pairs is related by any simple or obvious symmetry transformation.

How, then, does one characterize such an exotic type of symmetry breaking? It turns out that the way to do it is by examining the *relationships* among all the thermodynamic state pairs.<sup>7</sup>

This is a striking conclusion: it means that the nature of symmetry breaking in the spin glass is very different from anything seen before. Think back for a moment to the discussion in section 1.4 in which order parameters were introduced. Because they're thermodynamic variables, order parameters are functions of the microscopic state of a system. An experimentally obtained spin glass sample must be in one such thermodynamic state. So, following the usual practice, one should be able to identify an order parameter as a thermodynamic variable that refers *only* to that state, characterizing how it breaks the symmetry of the Hamiltonian. And yet the above discussion seems to indicate that this program, which has never failed for ordered systems, breaks down for the infinite-range spin glass. What does this mean? Can we not identify a macroscopic observable that characterizes a particular spin glass sample in a particular thermodynamic state?

The answer is no: at least for the SK spin glass, any attempt to carry out such a program is bound to fail. There is no adequate way to characterize the broken symmetry, or equivalently to define an order parameter, by referring solely to any single spin glass thermodynamic state. This cuts to the heart of what makes the SK spin glass so interesting, difficult, and novel all at the same time. We'll now plow ahead and attempt to extract the nature and meaning of the Parisi order parameter from all its

attendant complications, but keep the questions above in mind as we proceed.

### 5.6.1 The Spin Overlap Function

The problem is that although there are infinitely many thermodynamic states, statistically they all look alike; there's nothing special about any one to make it stand out from the others. Nevertheless, we can always assign arbitrary labels to the states; following convention, we'll use Greek indices  $\alpha$ ,  $\beta$ ,  $\gamma$ , . . ., to denote them. We'll also need to introduce a little notation:  $\langle \sigma_i \rangle_{\alpha}$  refers to the long-time average of the configuration of the ith spin in the thermodynamic state  $\alpha$ . To illustrate, suppose that in the state  $\alpha$ , spin number three has probability 3/5 of taking on the value +1 and probability 2/5 of taking on -1. Then

$$\langle \sigma_3 \rangle_{\alpha} = (3/5)(+1) + (2/5)(-1) = 1/5.$$
 (5.2)

We will use  $\tilde{\alpha}$  to denote the global spin flip of the state  $\alpha$ . In the example above,  $\langle \sigma_3 \rangle_{\tilde{\alpha}} = -1/5$  because  $\langle \sigma_i \rangle_{\alpha} = -\langle \sigma_i \rangle_{\tilde{\alpha}}$ . But for arbitrarily chosen, non-spin-flip-related states  $\alpha$  and  $\beta$ , in general,  $\langle \sigma_i \rangle_{\alpha} \neq \pm \langle \sigma_i \rangle_{\beta}$ .

Since there are no distinguishing features among the many spin glass states, how do we compare them? One way is to see how similar they are to each other, which can be accomplished by introducing a *spin overlap function*  $q_{\alpha\beta}$  between two thermodynamic states  $\alpha$  and  $\beta$ :

$$q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^{N} \langle \sigma_i \rangle_{\alpha} \langle \sigma_i \rangle_{\beta} . \tag{5.3}$$

From the definition of the EA order parameter, we see that  $q_{EA} = q_{\alpha\alpha}$  (and  $-q_{EA} = q_{\alpha,\bar{\alpha}}$ ); that is,  $q_{EA}$  can be interpreted as the *self-overlap* of a thermodynamic state<sup>9</sup> with itself. The

self-overlap depends on temperature (and field, if there is one); but when those are fixed, it is independent of thermodynamic state:  $q_{\alpha\alpha} = q_{\beta\beta} = q_{\gamma\gamma} = \cdots = q_{EA}$ . When  $\alpha$  and  $\beta$  are distinct, non-spin-reversed states, then it can be shown that  $-q_{EA} < q_{\alpha\beta} < q_{EA}$ .

## 5.6.2 Non-Self-Averaging and the Parisi Order Parameter

In the absence of anything else to grab on to, the spin overlap function provides a handle for investigating the nature of the low-temperature spin glass phase in the SK model. The presence of many thermodynamic state pairs at any  $T < T_c$ , where  $T_c$  is the temperature below which the spin glass phase is stable, raises the possibility that the distribution of overlaps could have a complicated form. This turns out to be the case, but what is also true—and surprising—is that it retains a lot of structure.<sup>10</sup>

Let's step back for a moment and see where we are. We're faced with a very large number (which goes to infinity as  $N \to \infty$ ) of thermodynamic states, any one of which the spin glass phase might settle into at a particular temperature below  $T_c$ . Statistically, they all look the same: they possess no spatial ordering, have zero magnetization, and all have the same self-overlap (equal to  $q_{EA}$ ). The only tool we have to compare them is the spin overlap function, and that can only compare two at a time.

Given all this, the sensible next step is to look at the *distribution* of spin overlaps at a given temperature. That is, suppose we have an N-spin SK spin glass in thermal equilibrium at temperature T. As we'll see in more detail later, the system might be found in any one of a large number of (pure) thermodynamic states, each with a well-defined probability, or weight, of occurrence. We'll use the symbol  $W_{\alpha}$  to denote the weight of state  $\alpha$ , with  $\sum_{\alpha} W_{\alpha} = 1$ . That is, if you measure the properties

of one of a large number of independent, identically prepared spin glasses all at the same temperature T and with the same coupling realization  $\mathcal{J}$ , you will find with probability  $W_{\alpha}$  that that particular system resides in state  $\alpha$ . The probability that two spin configurations chosen randomly and independently will have spin overlap between q and q+dq is therefore given by  $P_{\mathcal{J}}(q)dq$ , where the *spin overlap density*  $P_{\mathcal{J}}(q)$  is

$$P_{\mathcal{J}}(q) = \sum_{\alpha\beta} W_{\alpha} W_{\beta} \delta(q - q_{\alpha\beta}), \qquad (5.4)$$

where  $\delta$  is the Dirac delta (or  $\delta$ ) function,  $^{11,12}$  each sum of the double sum is over all thermodynamic states (so it includes all self-overlaps and their negatives), and the subscript  $\mathcal J$  indicates that the procedure is done for *fixed* coupling realization.

To get a feel for this function, we first examine its behavior in more familiar settings. In the paramagnet, there is a single thermodynamic state (with weight one), with all  $\langle \sigma_i \rangle = 0$ ; hence the spin overlap density is simply a  $\delta$  function at q = 0. The simple uniform Ising ferromagnet below  $T_c$  has two spatially uniform thermodynamic states, one with M(T) > 0 and the other with M(T) < 0. The magnetizations are equal in magnitude, and each state has weight 1/2. So there are four possible overlaps, and the overlap density is a pair of  $\delta$  functions, one at  $+M(T)^2$  and the other at  $-M(T)^2$ , each with weight 1/2, as shown in figure 5.2.

As already noted, in the SK spin glass, the overlap density has a more complicated form. There is an infinite number of states with self-overlap at  $q_{EA}$  (and the same with  $-q_{EA}$ ), but now there will also be many overlaps *between* these values. Lengthy analyses [3, 94–97] have shown that only a handful of thermodynamic states at low (but nonzero) temperature have weights that aren't extremely small, so the spin overlap function looks something like that in figure 5.3.

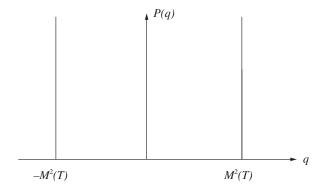


Figure 5.2. Spin overlap distribution for a uniform Ising ferromagnet below  $T_c$ .

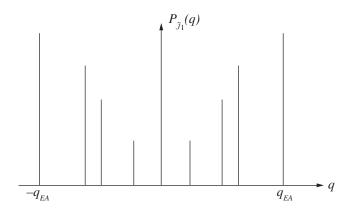


Figure 5.3. Sketch of the spin overlap density  $P_{\mathcal{J}_1}(q)$  for some large fixed N, low nonzero temperature, and coupling realization  $\mathcal{J}_1$ .

But that's not all. Surprisingly, it was found that *no matter* how large N becomes, the positions and weights of all overlaps strictly between  $\pm q_{EA}$  vary with the couplings  $\mathcal{J}$ . (The overlaps at  $\pm q_{EA}$ , on the other hand, are the same for all coupling realizations.) So a spin glass sample at the same T and with the same N but with

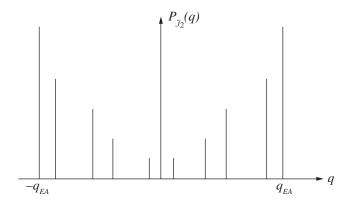


Figure 5.4. Sketch of the spin overlap density  $P_{\mathcal{J}_2}(q)$  for the same large fixed N and temperature as in figure 5.3, but with a different, independently chosen coupling realization  $\mathcal{J}_2$ .

a different coupling realization might display the overlap density in figure 5.4.

This is surprising, and also a little unsettling: in general, thermodynamics works because different samples behave the same way in the large-N limit. Here's a situation where sample-to-sample fluctuations of an important macroscopic property do *not* diminish as  $N \to \infty$ . This property is known as *non-self-averaging* and represents an important and distinguishing feature of the SK spin glass.

On closer inspection, non-self-averaging of the overlap distribution, though unusual, can be reconciled with our understanding of how thermodynamics should behave. The usual, measurable thermodynamic quantities—energy, free energy, magnetization (in a nonzero field), and so on—are in fact self-averaging in the spin glass. But as we pointed out in our discussion leading up to section 5.6.1, there's something intrinsically different about the Parisi order parameter, in that it is *not* a function of any single thermodynamic state. So we shouldn't be surprised

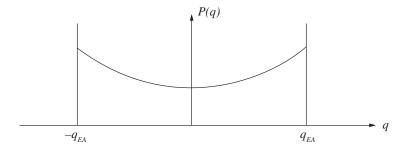


Figure 5.5. Sketch of the Parisi order parameter P(q).

that it doesn't correspond in any simple way to a macroscopic observable—in which case it needn't be self-averaging, either. The spin overlap, though important as a theoretical tool for understanding spin glass order, has no immediate or obvious observable consequences.

Given the non-self-averaging of  $P_{\mathcal{J}}(q)$ , the sensible next step is to examine its average over all coupling realizations:

$$P(q) = \int \prod_{1 \le i < j \le N} dJ_{ij} P(J_{ij}) P_{\mathcal{J}}(q).$$
 (5.5)

This is sometimes called the *Parisi order parameter*, sketched in figure 5.5. The nature of ordering in the SK spin glass phase is manifested by a typical  $P_{\mathcal{J}}(q)$  and the averaged P(q) taken together. The form of the latter indicates that no overlap value strictly between  $\pm q_{EA}$  is in any way special. Because those directly at  $\pm q_{EA}$  appear as  $\delta$  function spikes in *every*  $P_{\mathcal{J}}(q)$ , the Parisi function displays a continuum of values between the "goalposts" at  $\pm q_{EA}$ .

This is already quite a novel picture, but there's still one more surprise in store.

## 5.6.3 Ultrametricity

We mentioned earlier that the SK spin glass phase exhibits a good deal of structure, but so far what we've seen looks more like a complicated mess. Are there any further relations among the spin glass states?

At this point we've extracted about all we can from looking at overlaps between pairs of states. But that far from exhausts the possibilities, and when overlaps among *three* states are examined, a considerable degree of new structure is revealed: the space of overlaps of SK spin glass states is found to have an *ultrametric* structure [101]. To explain what this means, we need to digress briefly to explain the concept of a *metric space*.

An ordinary metric space is a set in which a distance, or metric, is defined between the elements (which we can hereafter take to be points). The ordinary three-dimensional space in which we live is a metric space, but the notion is more general. A metric space possesses a real-valued function d(x, y) for any two points x and y in the space. This metric function has the following properties (which we can easily see are satisfied by the physical space in which we live):

- 1.  $d(x, y) \ge 0$  (nonnegativity of distance);
- 2. d(x, y) = 0 if and only if x = y (self-explanatory);
- 3. d(x, y) = d(y, x) (symmetry); and
- 4.  $d(x, z) \le d(x, y) + d(y, z)$  (triangle inequality).

The last of these codifies the familiar notion that the sum of any two sides of a triangle is larger than the third. <sup>14</sup> Although these seem like very general and reasonable conditions (they are), they greatly restrict the possible types of spaces.

An ultrametric space is a special kind of metric space, replacing the triangle inequality with the *strong triangle inequality*:

$$d(x, z) \le \max(d(x, y), d(y, z)), \tag{5.6}$$

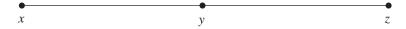


Figure 5.6. A configuration of three points that can occur in an ordinary metric, but not ultrametric, space.

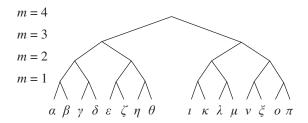


Figure 5.7. A simple, bifurcating ultrametric space consisting of 16 points.

Equation (5.6), where max (a, b) means the greater of a or b, seems a little inscrutable, but begins to make sense when presented in the equivalent form (which we leave as an interesting exercise for the reader) that any three points in the space form an acute isosceles or equilateral triangle. This immediately implies that any two points can have no third point in between; that is, an arrangement such as that in figure 5.6 cannot occur. To get from one point to another requires a single jump to that point; there is no sequence of smaller steps that can take you there.

What kind of space has this structure?

The answer: a nested (or treelike, or hierarchical) structure.

Take a look at figure 5.7. The points in the space, labeled  $\alpha$  through  $\pi$ , all live at the bottommost level. The distance between the points is defined to be the number of levels one must go up until their branches merge. So  $\alpha$  and  $\beta$  are at distance one from each other, as are, say,  $\lambda$  and  $\mu$ , while  $\beta$  and  $\epsilon$  are at distance three,  $\delta$  and  $\nu$  at distance four, and so on. Study the figure a little and convince yourself that a space defined this way satisfies the strong triangle inequality and is therefore ultrametric.

Everyone is familiar with at least one space having this structure, namely, kinship relations<sup>15</sup> among members of the same generation in a family tree. Here the distance between points is the minimum number of generations one has to go back to find a common ancestor. So in figure 5.7, points separated by distance one are siblings, sharing parents; those at distance two are first cousins, sharing one set of grandparents; and so on.

One of the most remarkable consequences of Parisi's solution is that spin overlaps among the spin glass states possess this property; that is, the function  $P_{\mathcal{J}}(q_1, q_2, q_3)$  for all pairs of overlaps among three states satisfies the strong triangle inequality [94, 95, 101].<sup>16</sup>

Space limitations prevent us from exploring this further, and we refer the interested reader to the references. It's worth noting, however, that one of the classic works on complexity [102, 103], to which we return in section 8.1.2, asserts that complex systems are built up through a hierarchical organization of their parts. It may be pushing too hard to say that the ultrametric structure of SK spin glass states is an example of this. But it's noteworthy that a hierarchical organization of states arises naturally from a structureless Hamiltonian; nothing is put in by hand. Whether this might be useful in complexity studies is an interesting question.

## 5.6.4 Summary of RSB

We can now put it all together and consider what we've learned about the spin glass phase of the SK model. The four principal features of RSB in the SK model in the  $N \to \infty$  limit are:

1. The spin glass phase consists of infinitely many thermodynamic state pairs, unrelated by any simple symmetry transformation.

- 2. The broken symmetry requires an infinite number of order parameters, which characterize the overlaps of pairs of states.
- 3. The overlap function displays non-self-averaging, that is, sample-to-sample fluctuations that remain significant no matter how large *N* becomes.
- 4. The distances between the states have an ultrametric structure.

This is a very pretty, even compelling, picture, and happily, some of its features, although not yet (3) and (4) above, have now been rigorously proved for the SK model [10,104–113]. Its vivid contrast with more conventional kinds of symmetry breaking—in particular, the noncorrespondence of the order parameter with any single thermodynamic state, and hence its nonobservability—marks the SK spin glass as one of the most interesting, and potentially important, statistical mechanical systems studied to date.

But does it apply to short-range spin glasses? Recall that our entire discussion in this section has been restricted to the infinite-range SK model. How generic is RSB? The answer is not completely known, but there have been advances in understanding this question over the past two decades. We'll return to this issue in chapter 7.

# 5.7 The Big Picture

At this point it's useful to step back and consider the larger picture that has been developed so far. We have already seen how, arising from what appear to be rather unremarkable and ordinary materials, a conceptual framework of great depth and profound mystery has begun to emerge. Some of the most fundamental questions—including whether there is a thermodynamic phase transition

to a new kind of low-temperature phase— have been answered for the infinite-range spin glass but remain unresolved for more realistic short-range models. Surely such a system would be of great interest to condensed-matter physicists and mathematicians interested in statistical mechanics—but why should complexity scientists be interested?

Let's recap some of the salient features that characterize spin glasses. First, like many real-world systems or problems, they're dirty. That is, they are defined first and foremost by the presence of quenched disorder. "Clean," well-ordered systems with well-characterized symmetries are, as we've seen, of fundamental importance in physics, but these features don't often carry over to complicated problems in the everyday world. In addition to disorder, spin glasses are highly frustrated systems: almost any realization of the couplings places numerous entangled constraints on the spins that are impossible to satisfy simultaneously. This is something that no doubt we're all familiar with in our everyday lives, but the sharp mathematical formulation of this property arising in spin glass physics lends itself beautifully to a number of complex, messy real-world problems.

As we've also seen, spin glasses possess a complicated state space structure, or "energy landscape," with many hills and valleys representing possible metastable or stable spin configurations. It is not yet known whether there are many "optimal" solutions, or ground states, in any finite dimension, and we return to this problem in chapter 7. But we do know at least that there are many metastable states of varying "near optimality." Many problems in computer science or biology or economics, for that matter, share these properties, and we will see in chapter 6 how these features can be mapped between spin glasses and problems from other areas of science.

We have also seen that the anomalous dynamical behavior of spin glasses—irreversibility, aging, memory effects—hints at

deeper layers of complex behavior that can reveal new insights and may be exploitable in mathematical or physical applications.

Perhaps most important, spin glasses, unlike glasses, possess a well-defined—if exceedingly difficult to solve—mathematical structure, starting from a simple-looking Hamiltonian containing built-in quenched disorder. This structure can be (and has been) exploited in applications to a variety of very different-looking types of problems. We have briefly explored, at a very simplified level, our mathematical understanding of the infinite-range spin glass, in which some of these layers of complexity have been peeled back and a rich and exotic structure of thermodynamic states has been found. Whether these features persist in more realistic short-range models is addressed in chapter 7. But for now it's worth noting that new mathematical techniques and physical insights that arose from attempts to "solve" the problem of spin glasses, whether infinite or short range, have found their way into a wide array of interesting applications. As we'll see in the next chapter, even without knowing these techniques in detail we can already obtain a glimpse of how spin glass ideas have been used to provide new ways of thinking about important problems in other areas of mathematics and science.

#### APPLICATIONS TO OTHER FIELDS

We've already encountered more than a few surprises yielded up by spin glass research. But perhaps none is so great as its unanticipated impact on an impressive array of problems from other fields. Mathematical and conceptual tools developed for spin glasses have found their way into a variety of applications, including the introduction of new methods for obtaining estimates on optimal solutions of computationally "hard" problems; the development of new algorithms with broad-based applicability; the development of new methods for biologically based computation; the develpoment of new models of neural networks, protein dynamics and folding, prebiotic evolution, and maturation of the immune response; and the elucidation of general features of rugged landscapes governing the dynamical behavior of these and other complex (and sometimes noncomplex) systems. In this chapter we provide an overview of some of the more successful and interesting of these applications.

# 6.1 Computational Time Complexity and Combinatorial Optimization

## 6.1.1 Combinatorial Optimization Problems

Combinatorial optimization problems reside at the intersection of computer science, mathematics, and engineering and range from pure mathematics (logic, graph theory, number theory) to practical applications (computer design, airline scheduling, data storage and retrieval), with a host of problems in between. We mentioned in the introduction one of the most easily described of these, the Traveling Salesman Problem (TSP), in which one seeks the shortest tour connecting a given collection of cities. Combinatorial optimization problems are characterized by a common set of properties: as the number N of variables (cities in the TSP, spins in the spin glass) increases, the number of possible solutions (tours in the TSP, spin configurations in the spin glass) grows explosively—at least exponentially in N and often faster. With each possible solution one can associate a cost function, which describes its "goodness": the length of a tour in the TSP or the energy of a spin configuration in the spin glass. The solution minimizing the cost function is called the optimal solution.

The study of combinatorial optimization problems constitutes an active research area for computer scientists, though their emphasis differs somewhat from that of physicists, mathematicians, or engineers who may be interested in some of these same problems. The latter might be interested, for example, in the average cost of the optimal solution as a function of the number N of input variables, where the averaging is over different realizations of the problem. In the TSP, N is the number of cities, and different realizations (also called instances) for a given N would constitute different placements of the cities within some fixed region.

The computer scientist, on the other hand, might be interested in different aspects entirely. An obvious one is to find the most efficient algorithm that solves *any* given instance of the problem. Needless to say, the physicist or engineer working on the same problem is probably very interested in this also, but may rely on the computer scientist to do the heavy lifting. Another, more theoretical research focus is to determine, or at least obtain bounds on, the computing time (as a function of *N*) needed by the most efficient algorithms to solve the problem, even if such algorithms are unknown. This last problem is interesting and important enough that we'll take a brief detour to discuss it more fully.<sup>1</sup>

## 6.1.2 Computational Intractability and NP-Completeness

With the advent of modern computers, previously unconsidered mathematical questions suddenly became interesting. Traditionally, mathematicians worried about things like whether a particular problem had any solution at all. If at least one solution could be proved to exist, then one typically wanted to know some of its properties: is it unique, how does it behave as some of the parameters of the problem are varied, and so on.

But now a new sort of question became important. For many problems of practical (and sometimes not so practical) interest, such as finding the shortest tour in a particular instance of the TSP, the existence of a solution is not in doubt. The \$64 K question now becomes *how long* it takes, under optimum conditions, to find the solution. In short, what is the "time complexity" of a given problem?

Of course, there are many possible ways to ask this question. You might want to know how long it takes to find the absolutely best solution, or simply one that approximates it to within a certain accuracy. You might need to know how long it takes an optimal algorithm to solve the "worst-case" instance of the problem, or you might be satisfied with knowing how fast a *typical* instance can be solved. Some might find a probabilistic approach suitable, others not. Here we'll briefly discuss what is probably the best known of these many variations: the question of whether "P = NP."

To describe this question, we need to sharpen some of our concepts. The *size* N of a problem is the number of input variables needed to specify a particular instance. For the TSP, this is simply the number of cities.<sup>2</sup> We can then define the *time complexity function* for a particular algorithm to be the *largest* amount of time (equivalently, number of steps) over *all* instances of size N that the algorithm requires to arrive at a solution. Notice that this way of defining time complexity effectively focuses on worst-case scenarios: it could be that an algorithm can solve the vast majority of instances of a problem in a time no larger than  $c_1N^2$ , with  $c_1 > 0$  some constant, but a very small number of atypical cases require a time  $c_2N^4$ . In that case the time complexity is nonetheless  $O(N^4)$ .

For a given problem, a *polynomial time algorithm* is then defined to be one whose time complexity is O(p(N)), with p(N) some polynomial function  $(O(N^c))$  for some constant c>0). If an algorithm's time complexity cannot be bounded by a polynomial, the problem is called *intractable*. While this could include algorithms that grow as slowly as, say,  $O(N^{\log N})$ , many known intractable problems have exponential time complexity. Some problems have been rigorously proved to be intractable; others have not but are suspected to be.<sup>3</sup>

To keep the discussion from getting too technical, we will informally define the classes *P* and *NP* in a model-independent manner, that is, without reference to encoding descriptions in terms of a "deterministic one-tape Turing machine" model.<sup>4</sup> It

will be understood that programs are run on the usual deterministic machines that we use every day. So a problem within class *P* is simply one for which there exists a polynomial time algorithm. The class *NP*, which stands for "nondeterministic polynomial time," is a little stranger, but in essence, a problem belongs to class *NP* if the correctness of a *guessed* solution can be computationally *verified* in polynomial time. The classes *P* and *NP* by no means exhaust all possibilities, but they do contain many interesting and important search and optimization problems drawn from graph theory, sequencing and scheduling, automata and language theory, statistical mechanics, number theory, logic, and many other areas.

Clearly, all problems in P are also in NP, but is the converse true? The question of whether  $P \subset NP$  or P = NP is one of the most important outstanding questions in theoretical computer science. A crucial step in the analysis of this problem was put forward by Stephen Cook in 1971 [116] with the introduction of the notion of NP-completeness.

This notion relies heavily on the idea of "polynomial time reducibility," in which one problem can be converted into another through an algorithm that is itself polynomial time. In other words, if problem  $\alpha$  is polynomial time reducible to problem  $\beta$ , then if  $\beta \in P$ , it follows that  $\alpha \in P$ . This is clearly a powerful tool with which to examine the structure of "algorithm space."

What Cook showed is that there exists a problem in NP, called the satisfiability problem [116], with the property that *every* problem in NP can be polynomially reduced to it. Therefore, if satisfiability belongs to P, then P = NP. On the other hand, if satisfiability is (as most experts suspect) intractable, then  $P \subset NP$ .

Cook went on to prove that there must be other problems in *NP* with this same property, and a year later, Richard Karp [117]

showed that a number of specific problems, including the TSP, were in this same category. The equivalence class of problems, including satisfiability, that are polynomially reducible to each other are called *NP*-complete; they are regarded as the "hardest" problems in the class *NP*. It is widely believed, but has never been proved, that *NP*-complete problems are intractable.<sup>6</sup>

At this stage you might be wondering what all this has to do with spin glasses. The answer is that there are several points of connection. At a practical level, spin glass concepts and techniques have been used to design algorithms and/or analytical approaches to approximately solve *NP*-complete problems (and also some in *P*); as should be clear by now, these represent a wide variety of important problems of both applied and theoretical interest. From a computer science perspective, it's also of great interest that the problem of finding the ground state of a three-(and higher-) dimensional EA Ising spin glass is itself *NP*-complete [119, 120].<sup>7,8</sup>

So spin glass mathematics can perhaps shed some light on combinatorial *NP*-complete problems. What about the other way around? Can the theory of *NP*-completeness, or the tools of computational complexity science more generally, help us solve any aspect of spin glass physics proper? Despite several attempts, the outlook at this point is discouraging. Perhaps the central issue is that statistical mechanics is interested in average or typical cases of a problem, but the theory of *NP*-completeness concerns itself, at least in principle, with (possibly atypical) worst cases.

But even if the two theoretical fields end up doing little for each other, spin glass research has provided impetus to the more practical problem of finding "good," if not the best, solutions, to many computational problems of widespread interest. And since computation is the main tool used in most complexity research, this is of no little import. It is to this subject that we now turn.

## 6.1.3 Statistical Mechanics and Combinatorial Optimization

Some similarities between combinatorial optimization and statistical mechanics are probably already evident. The input variables of combinatorial optimization problems are analogous to the statistical mechanical degrees of freedom introduced in section 1.2. For both, the number of possible assignments of values to all input variables grows explosively with their number. For ordinary statistical mechanical problems, the growth is exponential in the number of degrees of freedom N, while for combinatorial optimization, the growth is at least this fast, and sometimes faster: we've already seen that the number of tours in the N-city TSP grows as (N-1)!/2, which is faster than exponential. At a deeper level, the cost function in combinatorial optimization plays a role similar to that of the Hamiltonian in statistical mechanics: each provides a single number given an assignment of specific values of the N input variables, and this number provides a measure of the "goodness" of that particular assignment.

But there remain clear differences. One difference discussed in the previous section concerns the issue of worst case versus typical case. Another crucial difference is that in combinatorial optimization problems, one usually is interested only in the lowest-cost solution, or if that's not possible, one close to it. So even if one is willing to focus only on typical instances of a combinatorial optimization problem and not worry about rare worst-case outliers, there's still a fundamental difference with statistical mechanics. In the latter, the lowest-energy solution is thermodynamically relevant only at zero or very low temperature. More generally, one is interested in a temperature-dependent probability distribution over states, as discussed in section 1.5.

At this stage, there doesn't appear to be any natural fit for the notion of temperature in combinatorial optimization problems. Can the analogy between combinatorial optimization and statistical mechanics be exploited further? This question formed the basis of a classic paper by Kirkpatrick, Gelatt, and Vecchi [121], which suggested a very useful, statistical mechanics—inspired, algorithmic procedure for finding near-optimal solutions to a wide range of combinatorial optimization problems.

#### 6.1.4 Simulated Annealing

We've previously discussed how physical preparation of a ground state—or, more realistically, an equilibrium low-temperature state—of a material often entails more than simply cooling it down to a low temperature. In real life, the *process* of cooling is important; in particular, glass-formers and spin glasses tend to have relaxational and equilibrational timescales that grow rapidly as temperature lowers, and if the cooling is not done sufficiently slowly, the system will "quench" into a nonequilibrium, relatively high-energy state.<sup>9</sup>

To avoid such a high-energy, defect-ridden state, a sample is usually prepared through a process called *annealing* (see note 7 in chapter 2). In the specific example of growing a single crystal low in defects, this entails starting from a melt and lowering the temperature slowly—increasingly slowly as the temperature gets close to the freezing point, where most of the cooling time is spent. The idea of Kirkpatrick et al. is to follow a similar procedure computationally—that is, to use a process of *simulated* annealing. This requires introducing a fictitious "effective temperature" in the combinatorial optimization problem that would serve the same purpose as the real one in physical statistical mechanics: namely, to assign probabilities to different configurations according to their cost functions. One then slowly lowers the effective temperature, thereby finding low-lying states through a computational simulation of an annealing process. Several

algorithms can readily be used to implement this idea; among the best known, and the oldest, is the Metropolis algorithm [122].

The Metropolis algorithm was introduced in the 1950s to find equilibrium configurations of thermodynamic systems, such as a collection of atoms interacting according to a given Hamiltonian at some fixed temperature T. The basic step in the Metropolis algorithm is this: given some starting configuration at a given time step, a small change is proposed—for example, displacing a randomly chosen atom. This will cause a change  $\Delta E$  in the configuration energy, as computed through the system Hamiltonian. If  $\Delta E < 0$ , the change is accepted and the new configuration becomes the starting configuration of the next step. If  $\Delta E > 0$ , then the change is accepted with probability  $e^{-\Delta E/k_BT}$ . <sup>10</sup> Because this is just the Boltzmann factor introduced in section 1.5, it is not hard to show that the system will evolve under this algorithm from any starting point toward a Boltzmann distribution, that is, a system in equilibrium.

Notice that this algorithm allows the system to raise its energy (or cost function) at multiple steps. Why is this useful? For one thing, suppose that the system is "trapped" in some high-lying valley with relatively low barriers (see figure 4.7). The Metropolis algorithm allows the system to "climb out" of the valley, giving it the opportunity of finding a better valley at much lower energy. Since the temperature is artificial, how should it be chosen? If it's too high, the system will forever wander around numerous high-energy configurations, since there are so many more of them than low-energy ones. But setting the temperature to zero at the very start isn't a good idea either; it would result in a straight downhill run in energy. If the system starts from a random initial configuration, it would be overwhelmingly likely to get stuck in a high-lying valley.

Simulated annealing uses a Metropolis (or similar) algorithm to treat the combinatorial optimization problem as if it were a

physical sample to be annealed to low temperature. One starts from a high-temperature configuration (essentially, a randomly chosen list of input variables) and slowly lowers the effective temperature—that is, at each temperature step the system is allowed to equilibrate through the Metropolis algorithm—until no further changes occur. When this happens, the system is stuck in some local energy minimum—hopefully, a low-lying one. The rate of cooling is referred to as the *annealing schedule*, and is determined by the user. Simulated annealing establishes an appealing connection between combinatorial optimization and statistical mechanics.

At this point you might be saying that this is all very nice, but again, what has it got to do with spin glasses? This is where things get more interesting; the answer contains both general and specific aspects.

On the general side, note that much of spin glass behavior results from the combined influence of quenched disorder (section 4.4) and frustration (section 4.6). Both of these are fundamental aspects of many combinatorial optimization problems as well. How is that? Consider quenched disorder. There is only one instance of the uniform ferromagnet (all couplings equal and positive) or the uniform antiferromagnet (all couplings equal and negative). But there are (at least) exponentially many instances of an *N*-spin spin glass, each corresponding to a different coupling realization. Correspondingly, there are many instances of a combinatorial optimization problem with *N* input variables—for example, a list of the distances between all pairs of cities in the TSP.

Similarly, frustration in one form or another is present in many combinatorial optimization problems, although the definition is sometimes not as clean as in the spin glass. At a very general level, it manifests itself through the usual problem that a local rearrangement intended to lower the cost function in one region ends up raising it somewhere else. <sup>11</sup> If this weren't the case, it would presumably be a lot easier to find algorithms that quickly generated low-lying states.

The net effect is that the cost function of combinatorial problems typically has the sort of abstract "rugged landscape" structure presented by the energy landscape of spin glasses. Heuristically, then, it's easy for standard algorithms to get stuck in a relatively high-cost metastable state, and hard for them to find the much rarer low-cost solutions.

But these are all generalities. It's at the specific level that the analogy with spin glasses becomes most evident. To see why this is so, we briefly consider two examples, both discussed in [121].

#### Computer Design

The physical design of computers employs a hierarchical approach, in which circuits or groups of circuits are placed onto chips, the chips are arranged on a card, and the cards are arranged into higher-level packages. On a finer scale, these sorting tasks are subdivided into *partitioning*, in which a specific circuit is assigned to a particular chip; *placement*, which specifies the physical location of each circuit on its chip; and *wiring*, in which routing paths are determined for the wires that connect the circuits. Each of these procedures can be further resolved into subprocedures, but the basic outline of the overall process should be clear.

This must all be done in such a way as to satisfy geometric and spatial constraints while at the same time optimizing performance as a whole. In particular, the partitioning of circuits onto chips must ensure that they fit, while minimizing the number and length of wires crossing partition boundaries. The latter is particularly important because the number of signals crossing partition boundaries limits the overall speed of computation,

and to a lesser extent contributes to power consumption. At the same time, the more one reduces partition crossings, the more one tends to increase the congestion of circuit components on a chip. Qualitatively, at least, this is a classic example of frustration.

A simple model of this partitioning problem, as presented by Kirkpatrick et al., is as follows. Consider N circuits to be partitioned between two chips. The element  $a_{ij}$  of the connectivity matrix denotes the number of signals passing between circuits i and j. The two-valued variable  $\sigma_i = \pm 1$  indicates on which of the two chips circuit i is placed. So the excess of circuits on one chip over the other is  $M = \sum_{i=1}^{N} \sigma_i$  (formally similar to the magnetization in magnetic systems), while the number of signals crossing a chip boundary is  $\sum_{i < j} a_{ij} (1 - \sigma_i \sigma_j)/2$ . We want to minimize the "imbalance"  $M^2$  of circuits between chips as well as the number of crossings. This leads to a cost function

$$C = \sum_{1 \le i < j \le N} (\lambda - a_{ij}/2) \sigma_i \sigma_j, \tag{6.1}$$

where the parameter  $\lambda$  expresses the relative costs of imbalance and boundary crossings. If z is the average number of circuits connected to a typical circuit (analogous to the number of nearest neighbors to a given spin in a spin model), then choosing  $\lambda \approx z/2$  amounts to giving roughly equal weight to changes in imbalance of circuits versus. signal crossings.

Note that (6.1) is equivalent to an Ising spin model with short-range random ferromagnetic interactions (the  $a_{ij}$ 's) and a uniform long-range antiferromagnetic interaction (the  $\lambda$  term). If the  $a_{ij}$ 's are completely uncorrelated, then this system has spin-glass-like behavior at low temperature, with many comparable low-cost configurations.

The model described above is grossly oversimplified, but it provides a rough idea of how disorder and frustration can arise in

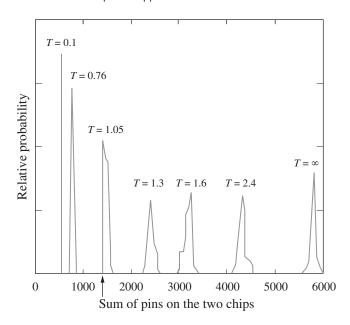


Figure 6.1. Results of simulated annealing in a two-way partition of a microprocessor using the cost function (6.1). Different temperatures are shown, and the arrow indicates the best solution obtained by a rapid quench from infinite to zero temperature. From [121].

diverse circumstances and how spin glass models and behaviors can arise in very different sorts of situations.

As an example, Kirkpatrick et al. used the logic design for a single-chip IBM 370 microprocessor, <sup>12</sup> which had about 5,000 primitive logic gates and 200 pins (corresponding to external signals). If one considers partitioning this system onto two chips, one can use a simulated annealing algorithm on a cost function similar to (6.1) to find the best partition (equivalently, number of pins). The results are shown in figure 6.1.

This can be further refined by considering placement (in which physical positions of the circuits are specified) and wire routing. We refer the interested reader to [121] for details.

## Traveling Salesman Problem

In the same paper, Kirkpatrick et al. used simulated annealing to find "good" solutions to the TSP with N cities arranged on a square of side  $\sqrt{N}$  (ensuring that the average distance between a typical city and its nearest neighbor was independent of N). Distances between cities were computed using a "Manhattan" metric in which the distance between two points is the sum of their separations along two perpendicular coordinate axes. Because real cities are not uniformly distributed in general but instead are clumped into relatively population-dense regions, the cities were randomly distributed inside nine distinct regions with empty gaps between them. Results at four temperatures for a 400-city problem are shown in figure 6.2.

It's interesting that even at relatively high temperatures, where small-scale details are entirely absent, some of the large-scale structure is already present: in particular, jumps between congested areas are rare and connect only nearest-neighbor regions. As the temperature lowers, the finer-scale structure within each of the congested regions begins to emerge.

The two examples briefly described above are the earliest applications of the simulated annealing algorithm, and remain instructive even now. Over the past 25 years, simulated annealing has become a standard simulation tool, used in a wide variety of problems (for a sampling of recent applications, see [124]; for a good review of older work, see [125]). Because it does have such broad applicability, it is not the best algorithm for any single problem; one typically requires specially designed algorithms tailored to a specific problem in order to achieve that. But for those looking for a general technique that arrives at a relatively good solution in a short time for a wide array of complex combinatorial optimization problems, simulated annealing is often the tool of choice.

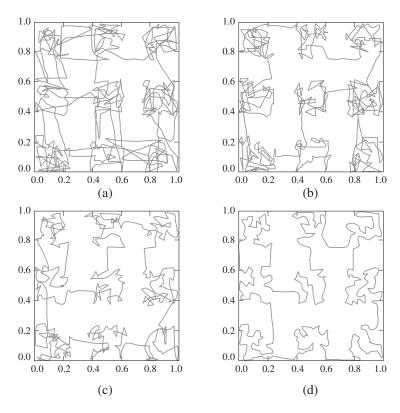


Figure 6.2. Results of simulated annealing at four temperatures in a 400-city TSP, with the cities uniformly distributed within nine spatially separated regions. Final temperatures are (a) T=1.2, (b) T=0.8, (c) T=0.4, and (d) T=0.0. From [121].

# 6.1.5 Analytical Approaches

Simulated annealing can be thought of as a practical tool that uses a spin glass analogy for solving hard combinatorial optimization problems whose cost functions display a "rugged landscape" structure. A more theoretical approach uses analytical techniques developed for the statistical mechanical analysis of spin glasses.

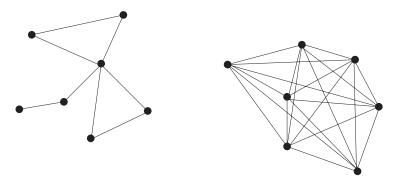


Figure 6.3. Two examples of graphs. The one on the right is a complete graph.

Here one is interested in calculating such properties as the average optimal cost, the structure of the solution space, the presence or absence of phase transitions as the effective temperature changes, and so on. A detailed discussion of these approaches and techniques requires applying technical methods, such as RSB, developed for analyzing infinite-range spin glasses, whose details are beyond the scope of this book. Here we intend merely to give a taste of the kinds of problems analyzed in this fashion.

We'll discuss in some detail an early and instructive example of this approach, due to Fu and Anderson [126]. They considered a problem known as graph partitioning, a version of which we encountered in the previous section. Graphs are generalized mathematical structures that model pairwise relationships between a collection of objects. Geometrically, they consist of a set of N points, called *vertices*, labeled  $V = \{v_1, v_2, \ldots, v_N\}$ , and a set of *edges*  $E = \{e_{ij}\}$ , where  $e_{ij}$  is a line segment connecting vertices  $v_i$  and  $v_j$ . Not all pairs of vertices need have edges connecting them; if all do, then the structure is known as a *complete* graph. Examples of graphs are shown in figure 6.3.

There are many variants of graph problems: lengths may be assigned to edges (in which case we speak of a *weighted* graph), or not, the graphs may lie in an ordinary Euclidean *d*-dimensional space, or not, the edges may be directed or undirected, and so on. Obviously, quite a few combinatorial optimization problems may be restated as graph theory problems, including the TSP (which is a weighted complete graph), the computer design problem, and the spin glass.

In the simplest version of the graph partitioning problem, the number of vertices N is even, and the problem is to partition the N vertices into two sets  $V_1$  and  $V_2$  of equal size such that the number of edges joining  $V_1$  and  $V_2$  is minimized. This is an NP-complete problem (see [127]).

Fu and Anderson studied a modified version of the problem in which each pair of vertices is connected with probability p independently of all other pairs. Using a spin glass analogy as before, one assigns the vertex  $v_i$  a value +1 if it belongs to  $V_1$  and -1 if it belongs to  $V_2$ . If a pair of vertices  $v_i$  and  $v_j$  has an edge  $e_{ij}$  connecting them, we assign the edge a value  $J_{ij} = 1/\sqrt{N}$ ,  $^{13}$  and otherwise  $J_{ij} = 0$ .

Because each set has an equal number of vertices,

$$\sum_{i=1}^{N} v_i = 0. (6.2)$$

The problem is then to minimize the cost function, which is related to a randomly diluted infinite-range ferromagnetic Hamiltonian

$$\mathcal{H} = -\sum_{1 \le i < j \le N} J_{ij} v_i v_j \tag{6.3}$$

by

$$C_N(p) = \mathcal{H}/2 + N(N-1)p/4$$
 (6.4)

under the antiferromagnetic constraint (6.2) [126]. The resulting frustrated system has spin-glass-like properties, which can be analyzed using techniques developed for infinite-range spin glasses. Fu and Anderson calculated the cost function and found excellent agreement with numerical results at N=200 and p>0.25 or so. <sup>14</sup> They also provided evidence of a phase transition in the solution space structure as effective temperature varies, with the critical temperature depending on p.

It is not our purpose here to emphasize the results or method of solution. Rather, we intend simply to show how graph-theoretic problems from entirely different fields of study have strong mathematical similarities with spin glass models, and how results from one area can shed light on the other.

A number of other combinatorial optimization problems have been studied using spin glass techniques, including the TSP (see [128]) and k-SAT (see [129, 130]). We refer the interested reader to the original papers for details.

# 6.2 Neural Networks and Neural Computation

The field of neural networks encompasses a wide variety of topics and models that range from those incorporating serious biology to those that are manifestly nonbiological. Although the latter are not terribly useful in understanding the biological brain, they can nonetheless provide general insights into the nature of cognitive processes such as memory and learning, and have led to new and useful biology-inspired computational tools. We provide a brief overview of some of these here; for a more comprehensive treatment, see, for example, the books by Hertz, Krogh, and Palmer [131] or Gurney [132].

#### 6.2.1 Historical Background

The modern study of neural networks spans nearly seven decades. In 1943 McCulloch and Pitts [133] introduced the concept of an "artificial neuron," a mathematical idealization that treated a single neuron as a binary logical unit: "on" or "off." This simple binary behavior is not characteristic of actual neurons, which can fire at different rates.

There are many ways of modeling the dynamics of McCulloch-Pitts neurons, but we will use the following simple choice. Let the state of the *i*th neuron at time *t* be denoted by the binary variable  $\sigma_i(t) = \pm 1$ , with +1 denoting an active, or firing, state and -1 an inactive one. This in turn is determined by inputs from *m* other neurons by

$$\sigma_i(t+1) = \operatorname{sgn}\left(\sum_{j=0}^m J_{ij}\sigma_j(t)\right), \qquad (6.5)$$

where we've taken time to be discrete,  $\operatorname{sgn}(\cdot)$  is +1 if its argument is positive and -1 if it's negative, and the "synaptic matrix"  $J_{ij}$  describes the effect of neuron j on neuron i:  $J_{ij} > 0$  corresponds to an excitatory interaction and  $J_{ij} < 0$  to an inhibitory one (and  $J_{ii} = 0$  for all i). The state of a neuron is determined by whether a weighted sum of inputs from connecting neurons exceeds—or doesn't exceed—a prespecified threshold; in (6.5) the threshold is zero.

The biological inspiration for this model is evident, but it should be clear that it is not meant to describe real neurons. McCulloch and Pitts did not provide specific formulations such as (6.5) of their model neuron; rather, it is one realization of their approach, and makes apparent the connection to spin glass mathematics.

The heart of McCulloch and Pitts's paper was a demonstration that any logical proposition can be encoded using their artificial neurons and that a dynamical network of them constitutes a universal computer: it can perform any computation that a Turing machine can. They therefore showed that a sufficiently large connective network (a "nervous net," in their terminology) among simple elements can give rise to arbitrarily complex finite propositions. As such, their paper represented a landmark in what was later to be known as complexity theory.

Soon afterward, Hebb [134] proposed a theory connecting neuronal activity to higher cognition. It viewed concepts as representations of patterns in the firing activity of a network of neurons and hypothesized that learning proceeded by synaptic modification (in the case of (6.5), of the  $J_{ij}$ 's) brought about by neural firing. Hebb's theory, and in particular his learning rule, had a profound impact on subsequent mathematical models of memory, learning, pattern recognition, association, and other cognitive tasks. The only one of the many examples of neural networks exploiting Hebb's ideas that we will discuss is the Hopfield model [135, 136], mostly because it connects closely with spin glass physics. Numerous other approaches are discussed in [131, 132, 137].

The final conceptual step leading up to the Hopfield model is the analogy with magnetic systems, which was first recognized explicitly by Cragg and Temperley [138, 139], who likened cooperative processes in the brain to those in ferromagnetic systems. This concept was modified and extended by several authors, including Griffith [140], Little and Shaw [141,142], and others. The connection to spin glasses, however, is most evident in the model proposed by Hopfield [135] in a foundational paper, to which we now turn.

# 6.2.2 The Hopfield Model

What Hopfield proposed in [135] was actually a new statistical mechanical model altogether, and as we shall see, it is interesting

not only for its applications to neural computation but also for its nontrivial thermodynamic properties. It clearly possesses spin-glass-like features and was surely inspired by the intense concurrent activity in spin glasses in the condensed matter community, but interestingly, in his paper spin glasses themselves are mentioned only briefly and in passing. However, mathematical tools borrowed from spin glass theory proved extremely useful in analyzing the Hopfield model. We'll turn to that aspect of the story in a little while. First, let's take a look at the model itself.

The subject of neural computation in general should be approached by asking, what does the brain do better than a standard digital computer? The answer is pretty much everything besides numerical computations. Pattern recognition, reconstructing memories or other data sets from noisy or partial or even incorrect information, learning, generalization, categorization of data, and many other tasks are performed faster and better by a small child than by the most massive computer with the most sophisticated software available to date (though perhaps not for much longer).

Hopfield begins by considering the problem of contentaddressable, or associative, memory. Consider the following familiar scenario: someone mentions the name of a friend of yours, and you instantly recall not just her features but the last time you saw her, what you had for dinner that night, what you discussed, and a myriad of other recollections. This train of thoughts will be largely unaffected if her name is mispronounced or gotten slightly wrong. So the problem is that of recovering a host of memories using partial and perhaps even incorrect information.

How can a model that performs the task of associative memory be constructed? The approach used by Hopfield, which is both intuitive and appealing, is to construct an artificial system whose state space comprises disjoint basins of attraction (see section 4.9) within which all noise-free dynamical flows converge to a fixed

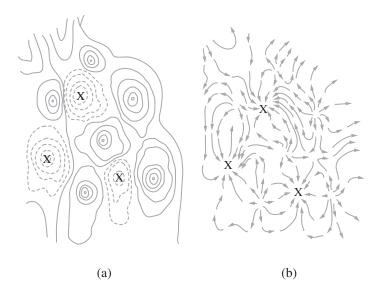


Figure 6.4. Sketch of a state space with three stable fixed points (denoted by x's) and their corresponding basins of attraction. (a) Energy contour map. (b) Dynamical flows with zero noise. From [143].

point (figure 6.4). It is easy to see that this solves, at least in an abstract sense, the tasks required of associative memory: the fixed points represent the complete and correct patterns, while all other points in the basin of attraction correspond to partial or slightly incorrect information. If the system lands in one of these basins, it quickly flows toward the stable attractor, that is, the fixed point representing the complete memory.

The question then is, how does one provide an actual example of a system that realizes this behavior?

Following Hebb's notion that a concept is a pattern of firing activities of a collection of neurons, and using the McCulloch-Pitts simplification of a neuron as either firing ( $\sigma_i = +1$ ) or not firing ( $\sigma_i = -1$ ), one can represent a pattern  $\mu$  comprising N bits of information by an N-component vector  $\xi_i^{\mu}$ , where

 $i=1,\ldots,N$ . If there are p patterns altogether, then  $\mu=1,\ldots,p$ . These will constitute the fixed point attractors of our system, that is, the "memories." Hebb's learning rule can be incorporated by choosing the connections among the neurons to be

$$J_{ij} = (1/N) \sum_{\mu=1}^{p} \xi_i^{\mu} \xi_j^{\mu}, \qquad (6.6)$$

so that learning a pattern  $\xi_i^{\mu}$  modifies the synaptic connections accordingly.<sup>16</sup>

However, there are at least two important differences between (6.6) and Hebb's ideas. The first is that nonfiring elements<sup>17</sup> modify the synaptic connection  $J_{ij}$  just as firing elements do. The second and more severe difference is that (6.6) implies that  $J_{ij} = J_{ji}$ ; that is, the effect of element i on element j equals the effect of element j on element j. Real neurons do not behave this way.

Part of the genius of Hopfield's model is the insight that such a manifestly nonbiological assumption is nonetheless extremely useful for biology-inspired computation. A symmetric "synaptic matrix" allows one to define an "energy function" for an arbitrary pattern  $\sigma = \{\sigma_1, \sigma_2, \dots, \sigma_N\}$ :

$$E = -\sum_{1 \le i < j \le N} J_{ij} \sigma_i \sigma_j , \qquad (6.7)$$

which has the same form as the zero-field SK Hamiltonian (5.1), but with the couplings chosen in a very different way. If we impose the zero-temperature dynamical rule of section 4.9 (i.e., when a given element  $\sigma_i$  is randomly chosen, its subsequent state is given by  $\operatorname{sgn}(\sum_{j=1}^N J_{ij}\sigma_j)$ ), then it is not hard to see from (6.7) that the system always runs downhill in energy.

An appealing picture is emerging wherein an imperfect input pattern  $\sigma$  will evolve toward the stored memory  $\xi^{\mu}$  that it resembles most closely, as in figure 6.4. However, this will be

true only if (1) the  $\xi^{\mu}$  are all fixed points of the dynamics, and (2) there are no other fixed points.<sup>18</sup> Unfortunately, for p > 1, neither of these is necessarily the case.

To see why, note that a configuration  $\sigma$  will be a fixed point if

$$\sigma_i = \operatorname{sgn}\left(\sum_{j=1}^N J_{ij}\sigma_j\right) \tag{6.8}$$

for all i from 1 to N. Using (6.6), we find

$$\operatorname{sgn}\left(\sum_{j=1}^{N} J_{ij} \xi_{j}^{\mu}\right) = \xi_{i}^{\mu} + (1/N) \sum_{j=1}^{N} \sum_{\nu \neq \mu} \xi_{i}^{\nu} \xi_{j}^{\nu} \xi_{j}^{\mu}.$$
 (6.9)

If the magnitude of the second term is smaller than one for all i, <sup>19</sup> then  $\xi^{\mu}$  will indeed be a fixed point of the dynamics, and the model will behave as intended, that is, as a model of associative memory. As we will see shortly, this will be the case if p is not too large.

There still remains the possibility of fixed points that are *not* the desired stored memories  $\xi^{\mu}$ . Unfortunately, these too exist and are known as *spurious states*.<sup>20</sup> One kind of spurious state consists of linear combinations of an odd number of stored patterns [145]. The second kind, which exists for sufficiently large p, is completely unrelated to any of the stored patterns, and these are sometimes called "spin glass states."

So the issue of how large p can be for the Hopfield net to serve as a model for associative memory—that is, where a correspondence exists between the memories assigned as input and the fixed points of the dynamics—becomes important. This maximum value of p is known as the network's *capacity*. Hopfield estimated that for p smaller than roughly 0.15N, recall would occur without significant error. Soon after, Amit, Gutfreund, and Sompolinsky [145–147] provided an analytical solution of the model that verified this estimate, and provided a fuller

understanding of its behavior for both noise-free and noisy dynamics.

Amit et al. treated the Hopfield net as an interesting statistical mechanical model in its own right, with a Hamiltonian given by equations (6.6) and (6.7). Aside from its intrinsic interest, studying the model at nonzero temperature provides information on its behavior under a noisy dynamics, similar to that given by the Metropolis algorithm (section 6.1.4).

Their first paper [145] considered the simpler situation of p fixed (at any finite value) as  $N \to \infty$ , and found a phase transition at  $T_c = 1$ : above  $T_c$  the system behaves like the usual paramagnet, while just below  $T_c$  the system evolves under the finite-temperature dynamics into an attractor state very closely correlated with one of the patterns (or its global flip). At even lower temperatures, below  $T \approx 0.46$ , new stable states appear; these are mixtures, or linear combinations, of the  $\xi^{\mu}$ . So it turns out here that a little noise is a good thing.

The harder and more interesting case is when p scales linearly with N:  $p = \alpha N$ . Here one needs to separate the cases of zero and nonzero temperature. For zero temperature, there is a sort of transition at a critical value  $\alpha_c \approx 0.138$ . When  $\alpha < \alpha_c$ , the Hopfield model works well as an associative memory: the system will fall into a pattern very closely correlated with a stored memory. When  $\alpha > \alpha_c$ , the error rate rises sufficiently rapidly that the system becomes useless as a model for associative memory (figure 6.5).

At nonzero T the model has an interesting phase diagram, as shown in figure 6.6. Below  $T_M$  the system will dynamically fall into metastable (section 4.9) patterns that are close to the stored memories. At  $T_c$  a phase transition<sup>21</sup> occurs, so that below  $T_c$  these patterns become thermodynamically stable.

There are additional structures uncovered by Amit et al.—the Hopfield model is quite rich as a statistical mechanical

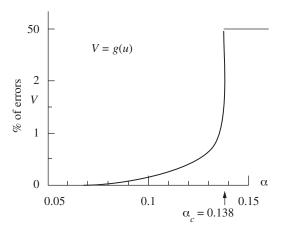


Figure 6.5. Average percentage of errors in the dynamically stable states as compared to the stored patterns as a function of  $\alpha$  for the Hopfield model at zero temperature. From [146].

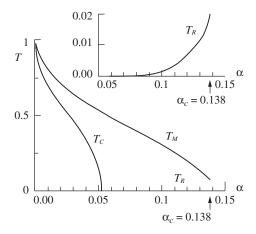


Figure 6.6. Phase diagram of the Hopfield model. Notations used are described in the text. The inset labeled  $T_R$  shows the line below which replica symmetry breaking occurs (section 5.6). From [146].

system—but we refer the interested reader to the references cited above.

The statistical mechanics of the Hopfield model were further investigated by a number of authors, most notably Gardner [148] and Gardner and Derrida [149], and its mathematical properties as a statistical mechanical model remain of great interest (see, e.g, [150–152]). Moreover, its robustness to the introduction of asymmetric couplings, correlated memories, continuous-output neural elements, learning with noise, and other modifications has since been explored (see [131, 137]). But at this point we leave the Hopfield net as a model for associative memory and turn to its uses as a means of neural computation.

#### 6.2.3 Neural Computation

The problem of recovering a complete memory on the basis of partial, fuzzy, or incorrect information is certainly an example of a computation, one crucial in our everyday lives. But what about mathematical problems, such as combinatorial optimization, that we ordinarily give to digital computers to solve? Can a highly interconnected neural network such as the Hopfield net be employed to solve those?

This question has been addressed by many authors; in the context of the Hopfield net, the foundations were set by Hopfield and Tank in a series of papers [136, 143, 153]. In designing such a computational device, they found it advantageous to drop the binary McCulloch-Pitts neural element in favor of a continuous-response element,<sup>22</sup> which enables performance of analog computations. This allows the processing elements to consist of simple electronic components, namely amplifiers, resistors, and capacitors.

The evolution of the system proceeds in continuous time. Using Hopfield and Tank's notation, if  $u_i$  is the input voltage

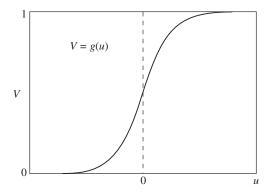


Figure 6.7. Input-output relation for continuous-response neural elements. From [143].

of the j th circuit element and  $V_j$  is its output voltage, then the nonlinear function  $V_j = g_j(u_j)$  characterizing its input-output relation will have the sigmoidal form shown in figure 6.7.

If  $T_{ij}$  is the conductance (i.e., inverse resistance) describing the strength of the "synaptic connection" between the output of element j to the input of element i, <sup>23</sup> and  $C_j$  is the capacitance of element j, then the system evolves in time according to

$$C_i \frac{du_i}{dt} = \sum_{j=1}^{N} T_{ij} V_j - u_i / R_i + I_i, \qquad (6.10)$$

which just expresses the conservation of electric charge.<sup>24</sup> Here  $R_i$  is the net resistance of element i and  $I_i$  is an externally supplied input current that sets a general level of excitability. A circuit that obeys (6.10) is shown in figure 6.8.

In the high-gain case (i.e., a steep curve in figure 6.7, approximating a binary function) with symmetric connections, the energy function of (6.7) holds near stable states, with the addition of a term reminiscent of the magnetic field term in the

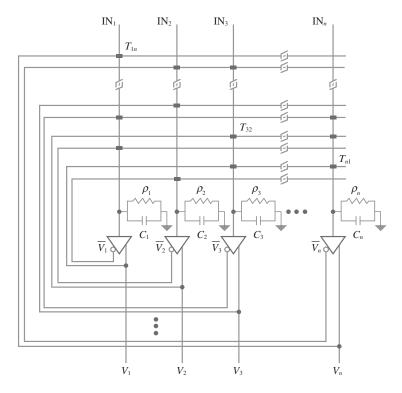


Figure 6.8. A model circuit obeying (6.10). Black rectangles represent connections with resistance  $1/|T_{ij}|$  between neural elements. A connection leading from a circle (representing an inverter) on the amplifier to an input of another represents an inhibitory ( $T_{ij} < 0$ ) connection; otherwise the connection is excitatory ( $T_{ij} > 0$ ). From [143].

#### SK Hamiltonian:

$$E = -(1/2) \sum_{1 \le i < j \le N} T_{ij} V_i V_j - \sum_{j=1}^N I_j V_j, \qquad (6.11)$$

and the state space structure and dynamics resemble those shown in figure 6.4. With a sufficient number of highly interconnected

neural elements, one can now build a versatile computing machine, one whose computational power grows with the number of such elements [153]. We describe one example of the capacity of this neural network to solve combinatorial optimization problems by turning to the now familiar example of the TSP.

We will follow the treatment given by Hopfield and Tank [143, 153], although more efficient versions of the same approach have been found [155]. Nevertheless, the basic ideas and flavor of the approach are well illustrated by the original proposal.

We therefore consider the circuit whose schematic is shown in figure 6.9. For an N-city tour, neuronal circuit elements are arranged in an  $N \times N$  array: the rows denote cities and the columns denote the order in which a city is visited in a tour. So a circuit element in row C and column 4 represents city C appearing as the fourth city visited in a putative tour. If this element is "on" (high-voltage state), then city C is the fourth city visited in the selected tour.

Because a city can appear only once in a valid tour, there must be inhibitory connections between all the neurons in a single row, and likewise in a single column, so that only one element can be "on" in any row and any column.<sup>25</sup> This is shown in figure 6.9, in which inhibitory connections are indicated. The "distance" between two cities can also be programmed through a choice of the synaptic coupling strength  $T_{ij}$ . Finally, since the voltage is near zero if an element is off, only a connection where both elements are on contributes to the energy.

The dynamical behavior of the system in state space starting from a random initial state will be similar to that shown in figure 6.4(b). If the circuit elements were binary McCulloch-Pitts neural elements, the computation would amount to a zero-temperature downhill run to the nearest minimum, leading to a high-"energy," nonoptimal tour; an example of this is

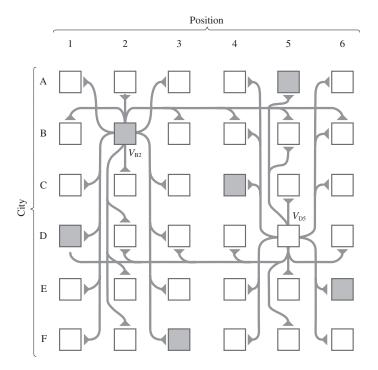


Figure 6.9. Sketch of neural network circuit configured to solve the TSP. Cities are indicated by letters and their positions in the tour are indicated by numbers. The pattern of synaptic connections is shown for only two elements,  $V_{B2}$  and  $V_{D5}$ . Connections emanating from the left and right sides of the boxes representing these two neurons are excitatory; all the rest (which connect neurons in the same row or column) are inhibitory. The chosen tour is indicated by the sequence of shaded elements; in the diagram, this is  $D \to B \to F \to C \to A \to E \to D$ . From [143].

shown in figure 6.10(c). The choice of analog, or continuous-response, neural elements allows the system to find a deeper minimum (figures 6.10(a) and 6.10(b)), just as the use of noisy, or finite-temperature, dynamics in simulated annealing can lead to deeper minima. The neural network doesn't use noisy

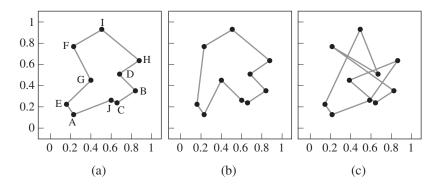


Figure 6.10. Ten-city tour, with the shortest path shown in (a). Both (a) and (b) were computed using continuous, or analog, elements. The path shown in (c) was computed using binary elements. From [153].

dynamics in the same sense as simulated annealing; rather, the analog nature of the neural elements allows the existence of intermediate states in which neural elements are neither fully on nor off, but instead can take on a continuum of values in between. Only the final state consists of all neurons either on or off.

As with simulated annealing, though, the system will eventually get stuck in some local minimum that is not the best possible solution. As noted earlier, it is usually the case that the best algorithm is one especially designed for a particular problem. The usefulness of approaches such as simulated annealing or neural networks is to provide a fairly general method for finding "pretty good" solutions in relatively short times for a wide variety of different problems.

To make this point explicit, figure 6.11 shows the comparative effectiveness of an analog neural network circuit and a specially designed algorithm. The tour in figure 6.11(b) was computed using the Lin-Kernighan algorithm [156], an especially fast and effective algorithm designed to solve the TSP.

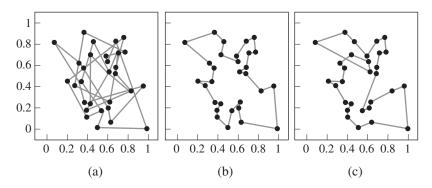


Figure 6.11. Thirty-city tour, with the shortest path shown in (b) (obtained using the Lin-Kernighan algorithm [156]). The tour shown in (a) is random, while the one shown in (c) was generated using an analog neural network. From [153].

Today, Hopfield-type networks continue to be used for a variety of problems, including pattern recognition [157], information retrieval [158], and others. As already noted, Hopfield nets are only one of a wide variety of neural network approaches to computing [131], but is probably the one that borrows most heavily from spin glass concepts.

# 6.3 Protein Folding and Conformational Dynamics

Proteins are the most diverse of the large biomolecules, serving a myriad of purposes. The enzymes are the best known: these are the proteins that catalyze the biochemical reactions that underlie the metabolism of every living organism. But proteins perform many other essential tasks as well. They play a central role in providing intra- and intercellular structure and support, are crucial in cell signaling processes, are responsible for muscle contraction, control the immune response, and carry out numerous other tasks.

The realization that spin glass concepts could be applied to protein dynamics and folding came a few years after their initial applications to combinatorial optimization and neural networks. The fundamental idea, though, had already been foreshadowed several decades earlier, with the notion that biologically active molecules should consist of matter organized in a state intermediate between a highly entropic liquid (which has insufficient stability for information storage and manipulation) and a rigidly ordered crystal (which has insufficient flexibility and adaptibility). Probably the most famous of these early insights is Erwin Schrödinger's<sup>26</sup> proposal, appearing in his 1944 treatise, *What Is Life?* [159], that the biological hereditary material is formed from "aperiodic crystals."

The problems of protein folding and fluctuations about the folded state (which we refer to as "protein conformational dynamics") are different from both a biological and a physical perspective. Although the process of folding precedes that of conformational dynamics, the application of spin glass techniques to the latter is somewhat easier to describe and was elucidated prior to the construction of spin glass theories of folding. We therefore begin by describing the problem of conformational dynamics.

# 6.3.1 Protein Conformational Dynamics

By the mid-1980s, experiments on compact, globular proteins such as myoglobin in the fully folded state exhibited a number of intriguing phenomena, some of which pointed to features we've encountered earlier: slow, nonexponential relaxation after a perturbation at low temperature, a multiplicity of intrinsic relaxational timescales, the presence of many metastable conformational substates, and several others suggesting the potential usefulness of a glass- or spin glass-type approach. Early studies

in this direction were initiated by Goldanskii and collaborators [160, 161], who proposed a glasslike model to explain the presence of "two-level systems" in proteins; Stein [162], who proposed a spin glass model that also used the notion of two-level systems to understand conformational substates and explain dynamics and fluctuations; and Frauenfelder's group [163], who emphasized the possible presence of hierarchical dynamics in explaining recombination experiments. We'll explain what all of these terms mean and how the various ideas relate to them, but first we take a brief detour to review some basic features of proteins relevant to the present discussion.

#### Levels of Protein Structure

A protein is a polymeric biomolecule consisting of a linear chain of amino acids, which are molecules containing an amine (NH<sub>2</sub>) group, a carboxyl (COOH) group, and a distinct side chain that distinguishes one amino acid from another. Biological proteins incorporate 22 different types of naturally occurring amino acids, with each protein identified through its *primary structure*, that is, its linear sequence of amino acids.

While this sequence ultimately determines a protein's properties and functions, it does so largely by determining its three-dimensional, or *tertiary*, structure. That is, a protein with a given primary structure will, at physiological temperatures and pH, "fold" into a highly specific three-dimensional conformation. A protein's *secondary structure*, as the name implies, is somewhere in between: it describes what might be thought of as localized spatial domains, that is, geometric configurations along partial segments of the overall molecule. In most proteins these come in one of two forms (though there are others): a single-helix structure known as the  $\alpha$ -helix and a pleated accordion-like structure known as the  $\beta$ -sheet.

## Conformational Substates and Myoglobin Dynamics

For a protein to carry out its specified biological role, it must be in its *native state*, that is, its "correct" tertiary structure. How a protein folds—that is, how it finds its native state given its initial primary structure—is an important and difficult problem known as the *protein folding problem*, which will be discussed in section 6.3.2. For now, though, we confine our attention to proteins already in their native states. We will focus on myoglobin, (Mb) which binds oxygen in the muscle tissues of most vertebrates.<sup>28</sup>

Myoglobin consists of 153 amino acids, with an iron (Fe)–containing heme group deep in the interior; it is here where the oxygen (O<sub>2</sub>) (or carbon dioxide [CO<sub>2</sub>]) molecule binds. The ligand (the molecule, in this case either O<sub>2</sub> or CO<sub>2</sub>, that binds to the heme group) is exceedingly small compared to the Mb molecule, which weighs roughly 16,700 daltons.<sup>29</sup> One might then imagine that it should be relatively easy for the ligand to diffuse into (or out of) the interior to reach the heme group for binding. This is not so, however; X-ray diffraction studies indicate that the molecule is tightly packed,<sup>30</sup> with most interstices between neighboring atoms much smaller than an O<sub>2</sub> or CO<sub>2</sub> molecule (see figure 6.12).

So how does the ligand diffuse into and out of the molecule? Because the average static conformation of the molecule won't allow ligand diffusion, there must be a dynamical component: the molecule is constantly *fluctuating*, or flitting between different conformational substates.

It is important to distinguish between these substates and the overall tertiary structure, or native state, of the protein. Broadly speaking, *all* substates correspond to the same tertiary structure, which for each given atom specifies its neighbors. Even so, there remains a certain amount of wiggle room, so to speak: while each atom—or in some cases a group of atoms—is confined to



Figure 6.12. Sketch of the three-dimensional myoglobin molecule, emphasizing both the secondary structure of the molecule, which consists of eight  $\alpha$ -helices, and the close packing of the molecule. The heme group where oxygen binds, actually deep in the interior, is also shown. From http://themedicalbiochemistrypage.org/hemoglobin-myoglobin.html.

a localized region of space, it may have some freedom to move around within that region. The question then becomes whether there exist many locally stable but distinct conformations, all with the same tertiary structure.<sup>31</sup>

#### Experimental Evidence for Conformational Substates

The earliest suggestions [165,166] that proteins such as Mb could exist in different conformational substates (with correspondingly different activation energies for ligand binding and dissociation) arose from both theoretical considerations and ligand rebinding

experiments (more on those momentarily). An important insight [165] was that the solvent in which the protein is immersed should play an important role in determining these substates. Because biologically active proteins don't exist in a vacuum, it is important to remember that one should think of the protein as a complex: the protein itself, its hydration shell (a several-molecule-thick layer of water adsorbed onto the protein surface), and the surrounding medium. All of these may, and probably do, interact to determine the protein conformational substates. So although for ease of discussion we shall usually refer only to the protein, it should be kept in mind that we're really referring to this complex.

In 1975, important experimental support for conformational substates was provided by Hans Frauenfelder's group at the University of Illinois, who performed a series of seminal experiments studying the dynamics of ligand binding to Mb at a variety of temperatures [167]. The basic idea was to dissolve the Mb in a solvent (usually but not necessarily glycerol-water) and introduce sufficient CO until most of the Mb molecules bound a CO molecule to the Fe in their heme group. At this point a short, strong laser pulse, with its frequency tuned so as to break the CO-Fe bond, was fired into the solution (a process called *flash photolysis*). Once the pulse ended, the CO usually found its way back to the Fe atom and reformed its bond, a process known as recombination. The idea of the experiment was to study the recombination kinetics; that is, at each fixed temperature the number N(t) of unrecombined molecules at time t was monitored.

If recombination were governed by a single activation barrier  $\Delta F$ , as in figure 6.13, one would expect at fixed temperature T an exponential decay of N(t):

$$N(t) = N_0 e^{-t/\tau(T)} (6.12)$$

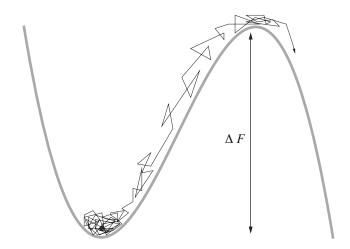


Figure 6.13. Cartoon of a simple barrier-crossing process representing thermal activation as the diffusion of a particle over a single barrier. We say "cartoon" because the relation of this picture to an actual barrier-crossing process is as a Road Runner cartoon to the theory of gravity; see http://www.youtube.com/watch?v=hz65AOjabtM.

with a timescale  $\tau(T)$  given by an Arrhenius law [168],

$$\tau(T) = \tau_0 e^{\Delta F/k_B T}. \tag{6.13}$$

Here  $\tau_0$  is a temperature-independent timescale whose order of magnitude is related to the frequency of escape attempts. For (6.12) to be valid,  $k_BT$  should be small compared to  $\Delta F$ .<sup>32</sup> And above roughly 220°K, exponential decay of N(t) is precisely what was seen.

Below this temperature, however, N(t) crossed over to a nonexponential decay. Between roughly  $160^{\circ}$ K and  $220^{\circ}$ K it took on a complicated form, and was interpreted by Austin et al. [167] as indicating that the ligand molecule encountered four successive activation barriers during the process of recombination. At even lower temperatures, between roughly  $40^{\circ}$ K and

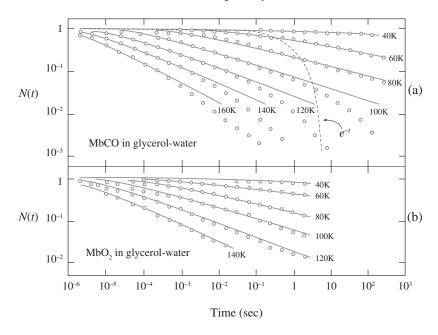


Figure 6.14. (a) Rebinding of CO to Mb after photodissociation. The solid lines are least squares fits to the data with  $N(t) = (1 + t/t_0)^{-\alpha}$ . (b) Rebinding curves of O<sub>2</sub> and Mb. From [167].

 $160^{\circ}$ K, N(t) simplified to an approximate power law:  $N(t) = (1 + t/t_0)^{-\alpha}$ , where the fit parameters  $t_0$  and  $\alpha$  vary smoothly with temperature. The experimental curves for both CO and O<sub>2</sub> recombination are shown in figure 6.14.

To explain the low-temperature data, Austin et al. [167] suggested two possibilities. The first was that below roughly 200°K, each Mb molecule complex froze into one of a large number of conformational substates, each with its own activation barrier (which should be sensitive to the detailed geometry in the vicinity of the heme group). This led to a "freezing in" of a distribution of activation barriers. Referring to this distribution

as  $g(\Delta F)$ , the formula for N(t) becomes

$$N(t) = N_0 \int d(\Delta F) g(\Delta F) e^{-t/\tau(T)}, \qquad (6.14)$$

with  $\tau(T)$  given by (6.13).

Note that (6.14) assumes that *each* molecule undergoes a simple single-barrier Arrhenius activation process. This assumption of a heterogeneous distribution of barriers, and hence recombination timescales, is known as *inhomogeneous broadening*. The other possibility is *homogeneous broadening*, where all molecules uniformly possess identical nonexponential relaxations.

To decide between these two possibilities, Austin et al. [167] performed multiple-flash experiments, in which the Mb solution was subjected to successive flashes before most molecules could recombine. If homogeneous broadening were occurring, then successive flashes would pump more ligands into states with longer escape times, and the recombination signal would get progressively weaker. If instead inhomogeneous broadening were occurring, then some molecules (those with longer rebinding times) would be removed from the picture entirely, but those with shorter times would continue to rebind. The absence of a progressive weakening of the signal at long times lent support to the assumption of inhomogeneous broadening.

Inhomogeneous broadening also fits nicely with the high-temperature data. At low temperatures, each protein is frozen into one of its many possible conformational substates, leading to a broad distribution for  $g(\Delta F)$  and therefore nonexponential relaxation. But the barriers are relatively low, and at higher temperatures each molecule has sufficient thermal energy to flit among its many substates, so each ligand-molecule complex now experiences a single average barrier that is the same for all. This would then recover the single exponential seen experimentally above  $220^{\circ}$  K.

We briefly discuss two additional pieces of evidence for conformational substates in Mb. The first comes from X-ray diffraction, which as mentioned earlier provides the average position of each (nonhydrogen) atom. But atoms are always in motion, causing attenuation of the X-ray scattering signal. This attenuation can be precisely related to the (temperature-dependent) mean square displacement  $\langle x^2 \rangle$  in the positions of the particles.<sup>33</sup>

Several factors can contribute to  $\langle x^2 \rangle$ ; an important one is always the vibrational motion of each atom about its equilibrium position, which of course has nothing to do with conformational substates. Additional contributions can arise from diffusion and rotation of atoms or groups of atoms, as well as other factors. And finally, conformational substates (if present) provide another source of attenuation of the X-ray signal. So the problem becomes one of teasing out the contribution, if any, from conformational substates—which, unlike vibrations, rotations, and so on, do not freeze out as the temperature is lowered. Consequently, a large temperature-independent displacement at lower temperatures should remain if conformational substates are present, and this in fact was found [169].

A related probe uses another feature of the solid state known as the Mössbauer effect [170], which is the resonant, recoilless emission (or absorption) of gamma-ray photons by certain atoms bound in a solid. In the case of Mb the isotope <sup>57</sup>Fe was used in the heme group as a probe. The recoil-less fraction of the Mössbauer transition is related, as before, to the mean square displacement, but this time of the iron nucleus only. This displacement was again found to be larger than that expected from vibrational fluctuations alone [171, 172].

# Proteins as "Disordered Systems"

We turn now to attempts to provide a theoretical understanding of these results. One problem in doing so is that while there are many ways to arrive at a distribution of relaxation times, it is difficult to devise tests to distinguish among them. Moreover, it is important to note that spin-glass-like ideas are not required to explain the data [173–176]. However, the similarity between conformational substates in fully folded proteins and the many metastable states of spin glasses is intriguing. It therefore seems worthwhile to search for an underlying model that can explain and unify many of these observations and ideas. We briefly examine such attempts.

Before doing so, we address a question that may—or should—be nagging the reader. Conformational substates make their appearance below roughly  $220^{\circ}$  K ( $-53^{\circ}$ C) in a glycerol-water mixture, where both the temperature and the medium are decidedly nonphysiological. So, even if such states are really there, what, if anything, is their relevance to biology?

It is entirely possible that there is none. But if such substates do exist—and experimental indications are that they do—then it's unlikely that they're irrelevant to biology. The low-temperature behavior of materials, whether biological or nonbiological, is generally relevant to their structure and functioning at higher temperatures as well. For ligand-binding proteins, we've already noted how dynamical fluctuations are crucial in the ligand migration process, which in turn is crucial for life in organisms utilizing these proteins. But what is the nature of these fluctuations? Presumably, they occur between conformational substates; so uncovering the nature of these substates may well have consequences for our understanding of the biological functioning of these proteins.

The emergence of these substates looks very much like the consequence of a system freezing into one of a large number of metastable configurations, separated by free energy barriers larger than the thermal energy. This "freezing-in" behavior is by now familiar: it has a glass- or spin-glass-like ring to it. But

of course, simply because something *looks* like a glass transition, and in a very restricted set of circumstances at that, doesn't prove anything. Can a plausible model with experimental consequences be constructed?

This was the aim of [162], which began by noting two important features of compact globular proteins such as Mb: first, Mb resembles a small disordered solid, and second, the three-dimensional structure is very closely packed (figure 6.12). The second point is clear from X-ray diffraction studies; the first is a little squishier. But if it captures anything meaningful about the protein, it should have a physical consequence. And it does: it predicts that there should be additional local degrees of freedom of a very specific kind. These are known as *two-level systems* (TLS), originally proposed by Phillips [177] and Anderson, Halperin, and Varma [178] to explain the anomalous low-temperature properties of glasses and spin glasses.

The idea is roughly that, owing to their lack of crystallinity, disordered materials such as glasses retain a degree of "floppiness" at the microscopic level: for example, although stuck within a localized region, atoms or clusters of atoms could still have different metastable positions between which they would continually flip. The precise nature of these TLS were unspecified, but they were shown to have an important consequence: among other things, they are responsible for a specific heat (section 1.6) that at low temperatures scales linearly with temperature.<sup>34</sup>

So, if the protein really could be modeled (at least in the restricted sense discussed here) as an amorphous solid, then TLS should exist in proteins, which has an observable consequence: their specific heat should have a linear contribution at low temperatures. Goldanskii et al. [160] measured the specific heats of various biopolymers (including DNA) and found this linear term, providing support to the protein-as-disordered-system viewpoint.

Based on these results, Goldanskii et al. separately proposed a glass model for proteins [160, 161].

Thus there appears to be a meaningful basis for considering proteins a type of disordered solid. But before proceeding, an important reminder is in order. No one suggests that proteins, the end product of millions of years of evolution, actually *are* a kind of glass or spin glass. They're far more complicated than that. The goal of the theoretical investigations described here is to show that *some* of the properties of proteins, primarily conformational substates, can be understood through glassor spin-glass-like modeling. They're certainly not crystals, so why couldn't nature take advantage of some of the features of noncrystallinity?

We now show how the second feature, the close-packing of Mb and similar proteins, enters into the picture. The model presented in [162] reasoned that the TLS in compact globular proteins could arise through local structures—amino acid side chains, perhaps some entire amino acids, or even a few small clusters of amino acids—having two or more metastable positions, corresponding to changes in bond angles (all the while being consistent with a single tertiary structure). Consequently, a single protein molecule will contain many TLS, and thus undergo many separate transitions at different locations. But a given TLS is unlikely to change its state independently of the others: movement of one from one local minimum to the other will, owing to the extreme close packing of the protein, result in a redistribution of other TLS nearby in space. Some of these redistributions would locally raise the conformational strain energy of the protein and some would lower it. These complex interactions among the shifting TLS serve as a kind of frustration.

This can be modeled through random interactions between different TLS. Expanding the conformational strain energy about its average  $E_0$  results in

$$E\{S^{(\alpha)}\} - E_0 = -\sum_{x} h_x S_x - (1/2) \sum_{x \neq y} J_{xy} S_x S_y + (\text{higher-order terms}),$$
 (6.15)

where  $S^{(\alpha)}$  refers to the entire protein in a specific configuration  $\alpha$ ,  $S_x = \pm 1$  refers to the state of a TLS at position x,  $S_x = \partial E\{S^{(\alpha)}\}/\partial S_x$ , and  $S_y = \partial^2 E\{S^{(\alpha)}\}/\partial S_x \partial S_y$ . Three- and higher-body interactions are assumed to be negligible (though in the unlikely event they are relevant, they wouldn't change the main conclusions). Because the interactions represented by the  $S_x$  are complicated and unknown, the simplest reasonable model assigns them a Gaussian distribution with standard deviation  $\tilde{S}$ :  $S_x$   $S_y$   $S_y$ 

If such a model is correct, then one would expect a freezing transition in the protein. This would not be a thermodynamic transition as discussed in section 1.6; a single molecule would have at most several hundred TLS, and possibly fewer. But this number is still sufficient for a meaningful (if nonthermodynamic) freezing transition to take place.

What can this say about recombination kinetics? With the assumption that  $h \ll \tilde{J}$ , and using the Gaussian distribution of couplings, we can now compute the distribution of the  $2^N$  possible conformational energy substates given N TLS, each of which interacts with z others on average:

$$P(E) = \frac{1}{\sqrt{zN\pi \tilde{J}^2}} \exp\left[-(E - E_0)^2/zN\tilde{J}^2\right].$$
 (6.16)

At temperature T, the probability D(E)dE of finding the protein with energy between E and E+dE is

$$D(E) \sim \exp\left[-(E - E_0)^2/zN\tilde{J}^2\right] \exp(-E/k_B T_0),$$
 (6.17)

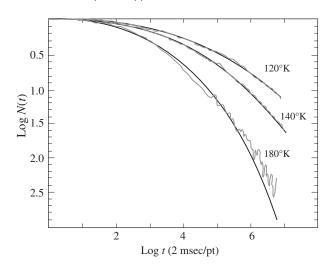


Figure 6.15. Recombination of T (tense structure) hemoglobin with CO after flash photolysis. For all curves, N=500,  $T_f=220^{\circ}{\rm K}$ ,  $E_0=4.5\,{\rm kcal/mol}$ , and  $\tilde{f}=0.1\,{\rm kcal/mol}$ . Fits were performed by R. Austin, J. LeGrange, and B. Tsuei, on data from R. Austin, J. LeGrange, and W. Cobau. From [162].

where  $\exp(-E/k_BT_0)$  is the Boltzmann factor introduced in section 1.6 and

$$T_0 = \begin{cases} T & \text{if } T \ge T_f \approx z\tilde{J}/k_B \\ T_f & \text{if } T < T_f. \end{cases}$$
 (6.18)

Here  $T_f$  is the effective "freezing temperature" below which the system is frozen into a conformational substate.<sup>37</sup>

This is useful, but it doesn't provide the distribution of free energy barriers  $g(\Delta F)$ . The simplest and most reasonable guess is that the distribution of activation energies follows the distribution of conformational strain energies in (6.17). Implementing this, one gets surprisingly good fits to the data, as shown in figure 6.15.

If these results were obtained only for Mb (or its close relative, hemoglobin), their generality might be suspect. Consequently, a series of more sensitive tests [179] was carried out on calmodulin, another compact globular protein of roughly the same size as Mb. Calmodulin binds calcium ions and plays a crucial role in a multitude of physiological processes. Instead of calcium, the experiment used the rare earth ion terbium, which has long emission lifetimes that are sensitive in a known way to the details of its environment. A glasslike transition was again found, with good agreement between theory and experiment. We refer the reader to [179] for details.

We close this section with an interesting proposal for Mb dynamics that suggests a hierarchy of free energy barriers [163, 180] in Mb recombination. The main idea was that structural relaxation in Mb following photodissociation proceeds through a type of hierarchical diffusion (see e.g., [181–185]) in state space. This diffusion was assumed to correspond to a physical process wherein as time proceeds, progressively larger motions occur when progressively higher barriers are overcome. There is consequently a series of increasing timescales that characterize the relaxation. Figure 6.16 describes this picture.

While the application of spin glass ideas to protein conformational dynamics is interesting, it may be that its most important contribution was to serve as a bridge to the even more interesting problem of protein folding, to which we now turn.

# 6.3.2 Protein Folding

Few would dispute that, just as physics underwent several profound revolutions in the early part of the twentieth century, so biology underwent its revolutions in the latter part of the twentieth century; the difference is that biology's revolutions

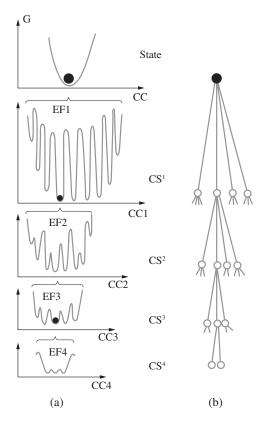


Figure 6.16. Schematic of hierarchical nesting of conformational states in Mb.  $CS^i$  stands for conformational substates at level i, CC for conformation coordinate at level i, CC for Gibbs free energy, and CC for equilibrium fluctuation. From [163].

have not yet abated. Biology's transformation began with the discovery of the structure of DNA in the early 1950s, which led quickly to identification of the mechanism by which it provided the blueprint for life: through the assembly of proteins that provide the structural and metabolic basis of all living organisms.

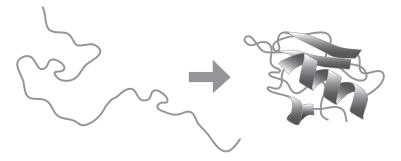


Figure 6.17. A generic sketch of the protein folding process. From http://commons.wikimedia.org/wiki/File:Proteinfolding.png.

Even so, a crucial feature of the story remains to be understood. DNA's instructions, as implemented through the cellular transcription mechanism,<sup>38</sup> determine the primary amino acid sequence of proteins. But as discussed in the previous section, a protein's function depends vitally on its tertiary structure. So before it can serve its intended purposes, the protein must "fold," or find its biologically workable three-dimensional structure; see figure 6.17. How does it do this?

Unraveling this process is by no means a trivial problem—in fact, it is considered one of the most difficult and important problems in molecular biology. Its importance lies not only in providing a key link in our fundamental understanding of how life works. The design of new drugs, the understanding of diseases resulting from misfolded proteins such as Creutzfeld-Jacob disease, "mad cow" disease, and possibly Alzheimer's, and many other applications of medical importance could potentially follow from a better understanding of protein folding.

## Levinthal's Paradox and Folding Phenomenology

It was realized early on that folding could *not* occur simply through a protein's randomly sampling a variety of possible

conformations until it hit on the correct one. In a brief paper that appeared in a conference proceedings [186], C. Levinthal noted that even a relatively small protein containing 150 amino acids would possess something of the order of  $10^{300}$  possible conformations. So even if a protein "tried on" each conformation in a picosecond— $10^{-12}$  seconds—it would take something of the order of  $10^{288}$  seconds to find its native conformation through random search. This is often referred to as *Levinthal's paradox*, although it's hardly a paradox, just a simple proof that the protein has to be employing a more nuanced strategy than simple random search. At the other end, it must also be more complicated than a straightforward "downhill run" to a minimum free energy state, which would result in folding times orders of magnitude shorter than those observed.

There is a vast store of phenomenology regarding the folding process, in fact far too much to be summarized here (for a good review, see [187]). We note only a few salient facts. A functional protein can be *denatured*—made to lose its correctly folded state—through either thermal or chemical means. Thermal denaturation is a primary reason why many organisms tend to survive only within a fairly narrow temperature range. <sup>41</sup> Proteins can also be denatured at physiological temperatures through changes in the chemical environment, a process known as cold denaturation. <sup>42</sup> Denaturation is often, but not always, irreversible, depending on both the protein and the means by which denaturation occurred.

# Thermodynamic Equilibrium or Kinetic Pathways?

The fundamental question to be addressed is *how* the primary structure determines the tertiary structure, given fixed temperature and pH. A natural guess would assert that the native state is a free energy minimum that is kinetically accessible from the unfolded state, the so-called "thermodynamic

hypothesis" championed by Anfinsen and others [188, 189]. If correct, then the folding problem should be susceptible to the tools of statistical mechanics.

But it could also be the case that the folded state does not correspond to a unique thermodynamic minimum but instead is reached through a series of easily accessible kinetic pathways. The presence of "chaperone proteins," which are needed for some proteins to fold correctly, is sometimes cited as evidence for this scenario (or at least against the thermodynamic hypothesis), but such proteins do not seem to affect the final state, and so the issue remains unresolved. In any case, any theory of protein folding must adopt, and at least a posteriori justify, one of these two approaches to the folding problem.

### The Principle of Minimal Frustration

One obvious difference between proteins and spin glasses is that proteins have evolved over millions of years; they're anything but random, haphazard collections of atoms. So it shouldn't be at all surprising that a protein's secondary structure, consisting of  $\alpha$ -helices,  $\beta$ -sheets, and other local configurations, does not conflict with its tertiary structure. This doesn't imply that frustration is completely absent; in a structure as complex as a folded globular protein, one should expect some residual conflicting constraints between some side chains trying to choose the local configuration that minimizes their energy, in a manner similar to that discussed in section 6.3.1.

This recognition of the role of evolution in protein design has been called by Bryngelson and Wolynes "the principle of minimal frustration" [190–192]: proteins have been "engineered" so that the primary sequence leads directly to secondary structures that favor the final, biologically useful folded state. The unavoidable remaining frustration has consequently been minimized.

Using this as a starting point, Bryngelson and Wolynes proceeded to write down a spin-glass-like energy for the protein consisting of three terms: the single-site energy associated with each amino acid (essentially the same as the first, single-spin term on the right-hand side of (6.15)); a secondary structure term, corresponding to nearest-neighbor interactions along the chain, and a third term corresponding to long-range interactions. This last term comes about because, in the folded state, amino acids far from each other along the primary sequence can have nearby spatial locations and thereby interact. Both the second and third terms have the same form as the second term on the right-hand side of (6.15), the difference being that the second term allows only interactions between neighboring amino acids along the primary sequence, while the third term allows for interactions between amino acids far separated along the chain but close in space. Bryngelson and Wolynes recognized that each amino acid or side group may have several possible locally stable configurations, so rather than the two-state Ising spin assumption made in (6.15), each degree of freedom can here take on several possible states.<sup>43</sup>

As we already know, such a Hamiltonian is exceedingly difficult to analyze. So instead, Bryngelson and Wolynes considered a simpler, qualitatively similar problem in which the energies of different protein conformations are taken to be uncorrelated random variables chosen from a distribution like (6.16). This "random energy model" results in thermodynamic features that are similar in some respects to those of more realistic spin glass models but are much simpler to analyze.<sup>44</sup> The model was first introduced by Derrida [194, 195], and it and its generalizations have since attracted a great deal of attention (for very recent work, see [196]).

Analysis of this model indicates that a solution of proteins can exist in several phases: a disordered phase in which many conformations are found, an ordered phase in which all proteins exist in the correctly folded state, and "glassy" phases in which proteins can be found in one of several misfolded states [190–192]. The last of these is especially interesting. Like more conventional glasses and spin glasses, there is frozen-in disorder, the dynamics are slow (section 4.3), and there is a great deal of metastability (section 4.9). <sup>45</sup> But what makes it interesting is its potential biological relevance: it has been interpreted as corresponding to the *molten globule* phase [201] of proteins.

The molten globule is a stable phase in which the protein is partially folded, with a free energy between those of the unfolded and native states. While some such states may correspond to misfolded "dead ends," their primary interest lies in the possibility of their playing a role as intermediates during the folding process. This result clearly merited further investigation, and ultimately led to a highly fruitful concept, that of the protein *folding funnel*.

### Folding Funnels

The application of spin glass concepts to protein folding leads naturally to consideration of the free energy landscape (section 4.9) that the protein explores during the folding process. At the beginning, when the protein is effectively a random coil, there is a great deal of conformational entropy, in accordance with the Levinthal paradox. As folding proceeds, however, the Levinthal paradox can be avoided if the protein can find pathways that lead to conformational energy reduction. In other words, folding can occur on reasonable timescales if the process is entropy-driven at early stages but at later stages is driven by conformational energy reduction. There will be barriers and false steps along the way; in particular, at intermediate stages, when the protein enters a glassy phase, metastable states are encountered as transient traps. Overall, though, the principle of minimal frustration implies that

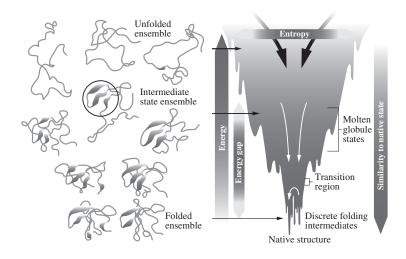


Figure 6.18. A sketch of the folding funnel, shown through a progression of structures (left) on a rough, funnel-shaped free energy landscape (right). From [204].

every conformation is connected kinetically to one further along the correct folding pathway.

The idea of kinetic pathways converging to the native folded state was beautifully captured by Onuchic and co-workers [202–204] through the concept of a rough "folding funnel," pictured in figure 6.18, in which a small number of energetic and entropic parameters provide a description of the global free energy surface. Of course, a realistic free energy landscape should be high dimensional, but the essential idea displayed in figure 6.18 is that there is a free energy gradient leading toward the correctly folded state. The roughness of the funnel indicates the presence of transient traps corresponding to local minima encountered during the folding process.

Requiring a folding funnel can be used to guide the construction of folding Hamiltonians; conversely, a proposed

Hamiltonian can be evaluated by examining whether, in combination with a suitable dynamics, it provides a funnel-like free energy landscape. Dynamics on these landscapes can then be studied to ascertain details of various steps that transpire during the folding process [204].

### Prediction of Protein Tertiary Structure from Primary Sequences

The principle of minimal frustration, the concept of folding funnels, and the general application of free energy landscapes and other spin glass concepts to protein folding provide a nice qualitative picture of the general features of the folding process and how the Levinthal paradox might be avoided. But are these ideas at all useful for prediction of tertiary structure, given a primary sequence? The answer, perhaps surprisingly, is yes, and the techniques are steadily improving.

A variety of approaches have been proposed; here we briefly mention only a few directly connected to the concepts discussed above, and refer the interested reader to the cited literature for details. One approach [205] has been to use Hopfield-like associative memory Hamiltonians (section 6.2.2), in which some of the vast store of experimentally derived folding phenomenology is exploited to encode the structures of a basis set of "memory proteins." Such a Hamiltonian is then used on a "target protein" that is, an amino acid sequence whose correctly folded structure is to be determined—and, using correlations between the target and memory proteins, predicts the folded structure of the former through minimization of the Hamiltonian. The success of this approach depends on the sequence homology (sequence similarity due to common evolutionary origins) between the memory and target proteins. Because of the glassy nature of intermediate states, simulated annealing (section 6.1.4) is sometimes employed [206]. This approach can be further refined through various optimization procedures; see [207].

A variety of other approaches based on optimization of an energy function have yielded steady improvement in predictive ability (e.g., for example, [208]). The field remains active to this day, and further developments in secondary and tertiary structure prediction from primary structure have changed the perspective on the protein folding problem from that of 25 years ago, when it was viewed as largely intractable, to today, when the problem is increasingly accessible to the methods of the statistical mechanics of quenched disorder.

### 6.4 Short Takes

Simulated annealing, neural networks, and protein folding and dynamics exhibit some of the most illustrative and interesting applications of spin glass concepts to complex systems. Not surprisingly, these represent only a portion of a wide-ranging array of applications. But the essence of a primer is brevity, and an extensive discussion covering this wide body of research belongs in a more comprehensive treatise. Nevertheless, we present here brief summaries of three other notable applications of spin glass theory to complex systems.

#### 6.4.1 Prebiotic Evolution

Few scientific problems capture our imaginations—and, more often than not, emotions—than the question of how life on earth came to be. And, as a problem in complexity, it is difficult to find a more stunning example of emergence. The principle of evolution via natural selection, understood within our modern notions of genetics and inheritance, provides a beautiful and comprehensive, if still unfinished, framework for understanding

how living organisms evolve and the workings of biology on earth. The transition from nonlife to life, however, presents a number of challenges that remain to be overcome. 46

In a famous book-length essay, Jacques Monod [211] argued that natural processes provide a sufficient underpinning for understanding the origin of life. Borrowing a phrase from Democritus, he attempted to show how a combination of random events (chance) and deterministic physical laws (necessity) could combine to give rise to the living world we see around us today.

In 1983, however, Philip Anderson [212], following a preliminary report [213], added a third element: deterministic chaos. His goal was to construct a model that could explain, within a statistical mechanical framework, the origin of biological information. Having no hope of reconstructing the actual events that led to the first information-carrying biomolecules, Anderson asked instead which conditions were necessary for transmissible, biologically useful information to arise at all—whether on earth or elsewhere. In other words, he sought a "universality class": a collection of systems that display the same essential behavior despite considerable differences in their microscopic constituents. For example, on earth almost all organisms use DNA to store and transmit information, but in other places (and perhaps on earth at much earlier times), other molecules could perform the same function:<sup>47</sup> here one is after how the ability to store and replicate information arose, not how the specific mechanism currently deployed on earth originated.<sup>48</sup>

In formulating this approach, Anderson suggested that any satisfactory model of prebiotic evolution must display the key features of *stability* and *diversity*. This requirement is most easily illustrated using a model containing only one bit of monomeric information, that is, one with only two types of monomer, an "A" and a "B," from which long polymeric chains can be built. Briefly put: by requiring diversity, one wants the synthesis

process to allow the construction of any of a large number of possible polymer end products, in a nonpredetermined way.<sup>49</sup> By requiring stability, one expects a particular end product, once selected, to be able to replicate itself and produce many copies over many generations.

It is easy to construct models that give one or the other feature but more difficult to find one that gives both. For example, if we assume that the A-B bond is strong compared to A-A or B-B, then outcomes  $ABABABAB \cdots$  or  $BABABABAB \cdots$  are the most likely, but then diversity is low—little informational entropy is generated.

Anderson's insight was to note that a natural way to generate both diversity and stability is to construct a survival function on the space of polymers that is a "chaotic random function" [212] of its arguments. A particular realization of this idea is to think of the monomers as Ising spins<sup>50</sup> and the survival function as a spin-glass-like Hamiltonian in a zero external field.<sup>51</sup> Given the rough landscape of such a survival function, there would be many possible but essentially unpredictable outcomes (corresponding to "landing" in one of many possible metastable states). Once a metastable endpoint is found, its stability properties would enable faithful replication over many cycles, though with a small error probability that introduces a type of noise that eventually drives the system from one metastable string to another (see fig. 6.13). The similarity to basic evolutionary processes is clear. Subsequent work extended this model to include the evolution of biological catalysis as well [218-220].

### 6.4.2 Kauffman's NK Model

Stuart Kauffman has worked in the area of complexity studies since before many of its current practitioners graduated from high school—in fact, long before the field became known as

complexity studies. Kauffman's long-standing interests include the search for a fundamental understanding of self-organization, selection, emergence, and adaptation; his unifying theme is the generation and increase of complexity. Given the ambitiousness of Kauffman's scientific agenda, it's not surprising that there exists a wide range of viewpoints on the validity of his ideas and speculations, but few would disagree with the assertion that he's one of the most original and creative thinkers in the field [16, 221–223].

One of Kauffman's undeniably important contributions is an analyzable model of a tunable rugged landscape, named (somewhat prosaically) the NK model [16,224–226]. In fact, the NK model turns out to be a generalization of a spin glass (though arrived at from an independent direction). As usual, N denotes the number of degrees of freedom in the system, which Kauffman imagined as amino acids in a protein, genes in a genome, and so on, while the tunable parameter K denotes the extent of interactivity of the system. Using genetics terminology, Kauffman described K as measuring the degree of epistatic interaction; that is, the extent to which the effects of one gene are affected or modified by others. Its meaning becomes clear using statistical mechanics language: if N is the number of spins, then K+1 describes the highest degree of spin couplings in a Hamiltonian or fitness function. That is,

$$K = 0 \Rightarrow \mathcal{H} = -\sum_{i} h_{i}\sigma_{i}$$

$$K = 1 \Rightarrow \mathcal{H} = -\sum_{i} h_{i}\sigma_{i} - \sum_{ij} J_{ij}\sigma_{i}\sigma_{j}$$

$$K = 2 \Rightarrow \mathcal{H} = -\sum_{i} h_{i}\sigma_{i} - \sum_{ij} J_{ij}\sigma_{i}\sigma_{j} - \sum_{ijk} J_{ijk}\sigma_{i}\sigma_{j}\sigma_{k},$$

$$(6.19)$$

and so on. The couplings  $h_i$ ,  $J_{ij}$ ,  $J_{ijk}$  (some of which may be zero) are typically taken to be random variables chosen from a well-defined distribution. So, if one is studying genomes, K=0 corresponds to a system where no gene interacts with any other, K=1 has each gene interacting directly with only one other (which returns us to the canonical spin glass), and so on, up to K=N-1, where every gene is epistatically affected by all the others. In this limit the landscape is completely uncorrelated; that is, a single spin flip can cause a large change in energy. Interestingly, the case K=N-1 corresponds to Derrida's random energy model [194, 195], described in section 6.3.2.

Since the NK model was constructed with biological applications in mind, one typically talks about "fitness" values rather than energies, with a local dynamics that drives configurations uphill rather than downhill,<sup>52</sup> but this is accommodated by a simple change of overall sign in (6.19). It is clear that the landscape is "smooth," or maximally correlated, when K=0: there is a single fitness maximum that is dynamically reachable from any starting configuration. As K increases, the landscape becomes less correlated and more rugged until, for large N and K, any local dynamical procedure is unlikely to find a local optimum that differs significantly from the overall mean fitness value.<sup>53</sup>

The tunability (through varying K) of the landscape is a useful tool for exploring the statistical properties of rugged landscapes that could be relevant for problems related to complex systems. Analytical results can be obtained for the extremes of K=0 and K=N-1, but otherwise, numerical investigations are generally required (but see [228, 229]). Kauffman and collaborators explored landscape properties, as a function of N and K, that included features such as the number of local optima, the mean length of a walk to the nearest optimum, the fitness distribution of optima, and so on.

Given its generality and flexibility, the *NK* model remains an active area of investigation, not only as a model for complex systems that evolve on rugged landscapes (see, e.g., [230]) but also as an interesting statistical mechanical system in its own right [229].

### 6.4.3 Maturation of the Immune Response

As is probably evident by now, one of the most powerful contributions that spin glass theory has made to the study of complex systems is the attention that it has focused on rugged landscapes; studies of dynamics on these landscapes have been useful in analyzing a variety of problems. In this section we briefly mention one more application, affinity maturation of the immune response.

This process shares much in common with biological evolution. Of course, the immune response involves a single individual rather than an entire species, timescales on the order of days rather than centuries or millennia, and somatic rather than germ cell mutations. But the essence of both processes centers on mutation and selection, and so mathematical models of walks on a rugged landscape that shed light on the evolution of species may also shed light on the immune response, and vice versa.

A complex organism responds to the invasion of foreign molecules (known as *antigens*, whether microbes or otherwise) by producing antibodies that bind to the antigen and subsequently eliminate it. The binding constant, or *affinity*, of antibodies to antigens increases with time, a process known as *maturation* of the immune response. The original antibodies made on first encounter with the antigen are encoded by genes inherited from the parents,<sup>54</sup> but as time proceeds, the antibody-coding genes mutate rapidly, producing antibodies with increasing affinity.

As the number of antibodies grows, they must compete for a scarcer supply of antigen, resulting in selection of those with the highest affinities.

While the *NK* and related models can be used to explore features of maturation of the immune response [225], other and sometimes simpler models, geared more specifically to this problem, have been proposed; see, for example, [231]. In recent years, similar ideas have been applied to HIV infection (see e.g, [232] and references therein). In the spirit of a short take, we forgo an extensive discussion here and refer readers to [233] for details.

# 7

# SHORT-RANGE SPIN GLASSES: SOME BASIC QUESTIONS

In this chapter we consider realistic spin glass models, in particular the Edwards-Anderson (EA) model introduced in section 4.5. Both the EA and the Sherrington-Kirkpatrick (SK) models are idealizations of the complicated spatial structure of spin-spin interactions in real materials, as discussed in section 4.4. In the EA idealization, the interactions are extremely short range, occurring only between spins that are nearest neighbors in the atomic lattice. This caricatures the actual spatial structure of laboratory spin glasses, but the EA model is nevertheless believed to distill their essential physics.

In contrast, the SK model is bereft of geometric structure and, as discussed in section 5.1, behaves like an EA model in the limit of infinite dimension. Of course, we're really interested in finite dimensions, so it's important to understand not only how the phenomena exhibited by the EA model depend on dimension *d*, but also how the similarities and differences between the EA and SK models depend on dimension. This chapter is devoted to

exploring some of the fairly deep issues involved in posing and answering these questions.

Although the nonequilibrium dynamics of spin glasses is of considerable interest (and was discussed briefly in section 4.3), we restrict our attention here to equilibrium thermodynamics. There the mother of all questions is whether there actually is a phase transition: as discussed in section 4.8, do realistic spin glass models undergo a sharp transition from a paramagnet to some sort of spin glass phase as temperature is reduced, and, in particular, does the spin glass phase display broken spin-flip symmetry?

We have already discussed how, for the SK model, the existence of a phase transition has been abundantly confirmed by numerical simulations, by nonrigorous analytical methods, and even by rigorous mathematical proofs. Much less has been confirmed for the EA model.

It is not too hard to prove that one-dimensional short-range systems, including spin glasses, do *not* exhibit phase transitions. For spin glasses in dimensions  $d \ge 2$ , we pretty much have to rely on numerical simulations. As noted in section 4.7, that evidence suggests that a phase transition occurs only for  $d \ge 3$  [78–80] (with the situation in d = 3 remaining unclear). At the moment, there seems to be no convincing theoretical argument as to why this should be so,<sup>1</sup> and the question remains open.

The existence of a phase transition in sufficiently high dimension (presumably  $d \geq 3$ ) is only the first of a series of important open problems concerning the EA model. Assuming there is indeed a spin glass phase at low temperature, the follow-up questions concern the nature of the transition and the behavior below the transition temperature. We focus here on the latter, with particular attention to the number of pure states, or phases, and how they are organized, as well as to the corresponding questions about the number of ground states. We've previously

described these concepts in a rough sense, but in order to proceed, we need to explore what they really mean.

## 7.1 Ground States

The notion of pure states, briefly mentioned in section 5.5, plays a central role in understanding the thermodynamic structure and behavior of spin glasses. In the more familiar settings of physical chemistry and materials science, pure states appear as gas, liquid, or crystalline solid phases. But as there is little familiar to grab on to in the spin glass setting, one is forced to rely on fairly abstract definitions and comparisons. We will do our best to make these notions comprehensible and user-friendly, and begin by considering the more straightforward situation of zero temperature, in which pure states are replaced by ground states.

In a finite-volume spin glass, the notion of ground state is simple: as already noted in section 1.4, it is the spin configuration(s) of least energy. To make things a little more precise, we'll denote by  $\Lambda_L$  a cube of side L, centered at an arbitrarily chosen point that we'll call the origin. We'll further define a finite-volume spin configuration  $\sigma_L$  to be a particular assignment of  $\sigma_x = +1$  or -1 for each site x in  $\Lambda_L$ ; clearly, for a  $\Lambda_L$  containing N spins, there are  $2^N$  such  $\sigma_L$ 's.

The energy of each  $\sigma_L$  is given by the EA Hamiltonian  $\mathcal{H}(\sigma_L)$  (equation 4.3). For simplicity, we hereafter set the external magnetic field h to zero.

As discussed in section 1.5, when a system is in thermal equilibrium at temperature T, the probability of a particular  $\sigma_L$  "appearing" is proportional to  $\exp(-\beta \mathcal{H}(\sigma_L))$ , where  $\beta = 1/k_BT$ . Let's now see what this implies. Its simplest consequence is that, if  $\sigma_L$  and  $\sigma_L'$  are two distinct finite-volume spin

configurations, with energy difference  $\Delta \mathcal{H} \equiv H(\sigma_L') - H(\sigma_L) > 0$ , then, as  $T \to 0$  (and hence  $\beta \to \infty$ ), the probability of  $\sigma_L'$  appearing is exponentially smaller, by a factor  $\exp(-\beta \Delta \mathcal{H})$ , than the probability of  $\sigma_L$  appearing. Clearly, as  $T \to 0$ , the only configurations surviving with nonzero probability are those whose energy is the absolute minimum possible (or at least tied for the minimum). This more formally establishes what we qualitatively noted earlier, namely, that ground states are the only relevant spin configurations at zero temperature.

Returning to the EA Hamiltonian, which in zero field is purely quadratic in the  $\sigma_x$  variables, we note that the energy  $H(\sigma_L)$  is unchanged if  $\sigma_L$  is replaced by  $-\sigma_L$ , the latter being the spin configuration (called the "global spin flip" of  $\sigma_L$ ) in which each spin variable  $\sigma_x$  of  $\sigma_L$  is multiplied by -1. This spin flip symmetry of the Hamiltonian implies that ground states always come in matched pairs  $+\sigma_L$  and  $-\sigma_L$ , related by a global spin flip. An interesting question is then whether there can be more than one ground state pair in a finite volume.

In fact, multiple ground state pairs *can* appear in finite spin glasses in certain cases, such as the  $\pm J$  model, introduced in section 4.5. For example, suppose  $\Lambda_L$  is a two-dimensional square with all  $J_{xy}$ 's equal to +J except for two couplings with  $J_{xy}=-J$  touching the origin, as in figure 7.1.

It is easy to see in this artificial case that there are exactly *two* ground state pairs with equal energy: one has all  $\sigma_x$ 's equal (either all +1 or all -1), while the other pair has all  $\sigma_x$ 's equal *except* the one at the origin. That is, the second ground state pair comprises the two spin configurations with all spins +1 except the one at the origin, which is -1, and its global flip. It is not hard to see that for other realizations of the  $\pm J$  model, there will generally be many ground state pairs of this type.

However, we're not particularly interested in these sorts of multiple ground state pairs, which differ only by local flips of

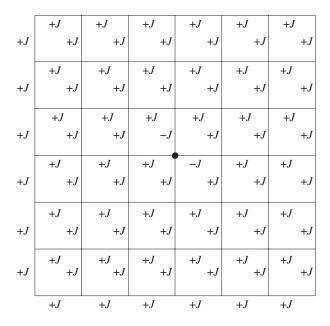


Figure 7.1. Illustration of the realization of the  $\pm J$  model described in the text. The origin is indicated by the filled circle.

spin clusters. By "local," we mean that any "zero-energy spin flip" that relates these pairs can be completely enclosed by a bounding surface whose diameter is small compared to the size of  $\Lambda_L$ . This sort of ground state pair multiplicity doesn't tell us anything profound about spin glasses; it occurs for relatively trivial reasons and is immediately understandable. It is simply a consequence of the *discrete* nature of the random couplings: in our example above, flipping the spin at the origin costs exactly zero energy. This can happen because all couplings have the same magnitude, differing only in sign.

On the other hand, for a *continuous* distribution of couplings, such as Gaussian (also discussed in section 4.5), such "local degeneracies" do not occur. That is, the probability that the sum

of the magnitudes of any *finite* set of couplings equals that of any other finite set is exactly zero.<sup>3</sup>

Because of this, there is zero probability that the flip of any finite set of spins has exactly zero energy, and so there can never be more than a *single* ground state pair in any finite volume. And because we're interested in general and universal features of spin glasses, and not those tied to a particular choice of coupling distribution (at least within the broad class of those with zero mean and finite variance), we should avoid working with specialcase models, such as  $\pm J$ , where local degeneracies occur. From here on, we'll confine ourselves to the Gaussian spin glass, in which local degeneracies don't occur and every  $\Lambda_L$  exhibits only a single ground state pair.

The question now becomes, what happens in *infinite*-volume systems? Here the situation becomes more complicated, and the question of ground state pair multiplicity becomes much more profound. Let's see why this is so.

Working with infinite volumes requires caution. The first concept that runs into trouble is that of "lowest-energy" configuration. It can be readily seen from (4.3) that the ground state energy magnitude scales linearly with the volume; given that, the notion of an infinite-volume spin configuration pair with "least energy" loses all meaning. There are at least two ways to address this problem, which may sound different but are actually equivalent, in that these two approaches result in exactly the same set of infinite-volume ground states.

The first approach focuses on *energy differences* rather than on the ill-defined total energy of an infinite system. The second approach takes an infinite sequence of finite volumes  $\Lambda_L$ , each of which has a unique ground state pair, and looks for convergence (in a suitably defined way to be described) of the ground states as  $L \to \infty$ . In this second approach, one looks at ground states before, rather than after,  $L \to \infty$ , and pretty much forgets about

the energies in the  $L \to \infty$  limit altogether. We'll now look at both approaches in greater detail.

In the first approach, one begins with an infinite d-dimensional lattice and asks whether a particular spin configuration pair  $\pm \sigma^*$  on it constitutes a ground state pair. The idea is relatively simple and eminently sensible: an infinite-volume spin configuration is a ground state if and only if there is no flip of any finite subset of spins that lowers its energy. Here one is looking only at the difference in energy of two infinite-volume spin configurations, chosen to be identical except for a finite number of spins. Their difference in energy is therefore finite and perfectly well defined,<sup>5</sup> and moreover must be either strictly positive or negative in the Gaussian spin glass.

Before discussing the second way of defining infinite-volume ground states, we can now formulate the interesting (and still open for  $d \geq 2$ ) question about numbers of ground states: for an EA spin glass with Gaussian couplings, is there more than a single infinite-volume ground state pair? This is a sensible question even when each *finite* volume has only a single pair, and it is one that is not at all easy to answer in general dimension.

However, it *can* be confidently answered in one dimension. Here there is only a single ground state pair on the infinite line, namely, the spin configurations in which each coupling is *satisfied* (section 4.6).<sup>7</sup> To generate a ground state, all you need to do is pick the spin at the origin to be either +1 or -1 and then work to the right, assigning the sign of each new spin you encounter so that it satisfies the coupling on its left. At the same time, work your way to the left using the same procedure (except that now each time you satisfy the coupling to your right).

To see that no other ground states are possible, consider first the situation where there are two or more unsatisfied couplings in a putative ground state. The reader should check that in such a spin configuration, one can pick two such unsatisfied couplings and flip all of the spins between the two. This will clearly lower the energy.

To show that a spin configuration with a *single* unsatisfied coupling is not a ground state requires a slightly more refined argument. Suppose the unsatisfied coupling connects sites n and n+1 (measured from the origin), and suppose that this coupling has magnitude  $|J_{n,n+1}|$ . Because the couplings are chosen independently from a Gaussian distribution, it must be that if one looks far enough to the right (or left), one can eventually find a coupling  $J_{n',n'+1}$  of smaller magnitude, that is, with  $|J_{n',n'+1}| < |J_{n,n+1}|$ , and then a flip of all the spins in between *these* two couplings will lower the energy, even if  $J_{n',n'+1}$  was satisfied before the flip and is unsatisfied after.

We now turn to the second way of defining infinite-volume ground states. Here one considers limits of finite-volume ground states on  $\Lambda_L$  as  $L \to \infty$ . To understand this procedure properly requires some elaboration, beginning with the notion of a "boundary condition" on a finite volume.

Note that spins on the boundary of any  $\Lambda_L$  are special in that they live in a different environment from the interior spins. Figure 7.2 illustrates this in two dimensions.

In figure 7.2 all of the interior spins, connected by lighter couplings, have four neighbors each. The boundary spins, connected by darker couplings, have three neighbors if they live on an edge and two if they live at a corner. Because of the special nature of the boundary, we need to specify how its spins behave.

One possibility is to fix the value of each boundary spin, say by flipping a fair coin and assigning it the value +1 if the coin comes up heads and -1 if it comes up tails. These boundary spins thereafter remain fixed, while the interior spins can take on any configuration, and so we refer to this as a "fixed" boundary condition. The number of distinct fixed boundary conditions for a particular volume is  $2^{N'}$ , where N' is the number of boundary spins.

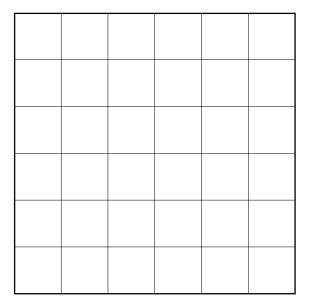


Figure 7.2. A finite square in two dimensions. Sites on the boundary, denoted by the dark line, have fewer nearest neighbors than the interior sites.

Another possible boundary condition—denoted, reasonably enough, as the "free" boundary condition—is one in which the boundary spins are allowed to take on any values they want, without restriction. However, the boundary condition used most frequently is one requiring each boundary spin to take the same value as that of the boundary directly opposite it, as illustrated in figure 7.3.8 This is called the "periodic" boundary condition.

The nice thing about the periodic boundary condition is that, by identifying spins at opposite sides of the volume, boundary spins behave like interior spins; all effectively have the same number of nearest neighbors. As a consequence, periodic boundary conditions minimize boundary effects and hence are

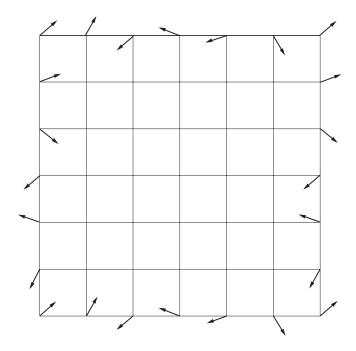


Figure 7.3. A boundary configuration obeying periodic boundary conditions, in which each (non-Ising) spin is identified with the spin at the opposite boundary point. Note that the spin at all four corners is the same. Periodic boundary conditions means that any pair of boundary spins on opposite sides can take on any allowed value, but they must be the same.

often used both in numerical and theoretical studies of the EA model.

We can now discuss what we mean by the "convergence" of an infinite sequence of finite-volume ground states. Let's consider a sequence of  $\Lambda_L$ 's, with  $L \to \infty$  in some fixed dimension d. For example, we might consider the sequence of d-dimensional cubes centered at the origin with  $L=10^4, 10^5, 10^6, \ldots$  For each of these we need to specify a boundary condition—in this particular

example, let's say periodic for all. Then each volume will have its own unique ground state pair, denoted by  $\pm \sigma_I^*$ .

We now focus on a fixed, finite region—we'll refer to it as a "window"—say, the cube with side length 3,000 centered at the origin [239]. Let's denote by  $\sigma^w$  the spin configuration pair restricted within this window; in other words, we look only at what the spins are doing inside the window and ignore all those outside. As the sequence of  $\sigma_L^*$ 's changes as L increases,  $\sigma^w$  will also change, at least for a while. Eventually, however, when L gets large enough and the boundaries are sufficiently far from the window,  $\sigma^w$  may settle down to a final, unchanging state. If so, the ground state spin configuration pair in that particular window has converged.

That's a start, but it's not enough. We next have to look at a window of size 30,000 (say), and do the same thing. <sup>10</sup> If the sequence of  $\sigma_L^*$ 's settles down to a unique spin configuration pair within that *new* window, we increase the size of the window again and repeat the procedure. We say that an infinite sequence of finite-volume ground state pairs converges to an infinite-volume ground state pair if and only if the spin configuration pair in any finite window, no matter how large, settles down to a limiting pair.

While performing this procedure one has the freedom to choose any boundary condition one wants, for any volume. One might choose a fixed boundary condition for one volume, a different fixed boundary condition for another volume, and so on; or instead, one might prefer periodic boundary conditions for some volumes and free boundary conditions for others, and so on. The possible choices are unlimited. For brevity we define a "sequence" to mean an infinite sequence of volumes, each with a specified choice of boundary condition.

In light of this enormous freedom, one might expect that most sequences would *not* converge to an infinite-volume ground state. And this may well be true. But at the same time, one can prove

mathematically<sup>11</sup> that at least *one* such sequence will converge to an infinite-volume ground state pair. The question now becomes, are there different sequences leading to *distinct* infinite-volume ground state pairs?

The freedom of choosing boundary conditions in the second approach guarantees that both approaches give rise to exactly the same set of infinite-volume ground states. This is not immediately obvious, even in the 1D Gaussian spin glass. Here's why. Suppose you decide on the following boundary condition, which you're perfectly free to do: for each L, the product of the two chosen boundary spins is -1 if there is an even number of negative couplings and +1 if there is an odd number. This will guarantee (think about it) that the finite-volume ground state for each L will have exactly one unsatisfied coupling. So shouldn't the limiting ground state pair on the infinite line have exactly one unsatisfied coupling, which we asserted above is *not* an infinite-volume ground state in d=1?

Here's where the utility of using windows comes in. To be a finite-volume ground state, that unsatisfied coupling must be, in each finite system, the one with the *smallest* magnitude. A little thought will we (we hope) convince the reader that, as *L* continues to increase, the location of this "weak link" will move out to infinity (randomly, sometimes way off to the left and sometimes way off to the right). So the limiting spin configuration will not have *any* unsatisfied coupling since in every finite window it will eventually settle down to the one where all couplings are satisfied. A picturesque but useful way of visualizing this is to think of the location of the unsatisfied coupling as "wandering off to infinity": it eventually moves outside any window.

The upshot is that in one dimension, where frustration is absent, both approaches lead to a single ground state pair, in which all couplings are satisfied. Frustration, however, changes

the game for spin glasses when  $d \ge 2$ ; now *every* spin configuration, ground state or not, must have unsatisfied couplings. But in spite of the fact that one dimension is very different from two or more dimensions, the analysis we have just done for d=1 is surprisingly instructive for higher dimensions. How should we think of the problem of ground state multiplicity in those?

The most useful approach is to compare two different spin configuration pairs,  $\pm \sigma$  and  $\pm \sigma'$ , by looking at the collection of *couplings* that are satisfied in one and not the other, that is, couplings connecting nearest-neighbor sites x and y with  $\sigma_x \sigma_y \sigma_x' \sigma_y' = -1$ . We call the collection of all such couplings the *interface* between the two spin configuration pairs.<sup>12</sup>

We can now reframe the question of whether there exist multiple ground state pairs: Are there different sequences of boundary conditions such that the interfaces between their ground states do not wander off to infinity as  $L \to \infty$ ? If so, there exists more than one ground state pair. An equivalent test is to ask whether changing boundary conditions arbitrarily far away can change a satisfied coupling in a fixed window to unsatisfied, or vice versa. If the answer is yes, no matter how far away the boundaries are, then there are multiple ground state pairs, otherwise not. A little reflection should convince the reader that all these ways of framing the issue are equivalent.

Whether any of this actually happens is an open problem for all dimensions  $d \geq 2$ , although there is considerable evidence, both numerical [242, 243] and analytical [240, 241, 244], that at least in d=2, the answer should be no. And in higher dimensions, the issue is quite unsettled and interesting. At this time, there are competing nonrigorous arguments leading to opposite conclusions, as we discuss later in this chapter.

Such is also the case for pure states at low but nonzero temperature, as we discuss next.

### 7.2 Pure States

Phase transitions in a material like  $H_2O$ , which changes from a liquid to a gas as temperature increases, are modeled by studying how the thermodynamic state (section 5.5) changes as the transition temperature is crossed. Just like ground states, thermodynamic states are easily defined in finite volume with a specified boundary condition. We mentioned earlier that the probability of a configuration  $\sigma_L$  with energy  $\mathcal{H}(\sigma_L)$  is proportional to  $\exp(-\beta\mathcal{H}(\sigma_L))$ . A finite-volume thermodynamic state is then simply an assignment of these probabilities to every finite-volume spin configuration (each of which must obey the boundary condition).

What about infinite volume? As before, dealing with this case is more involved, but it's unavoidable if we want to explain phase transitions and the precise meaning of pure states (which correspond above to liquid water or gaseous water vapor).

Why is that so?

One answer is that nonsmooth changes in a material in thermal equilbrium (like the discontinuous jump in density from gas to liquid, or the sudden release of heat as water freezes to ice) cannot strictly occur (mathematically speaking) in a finite system. *All* thermodynamic functions in a finite system, regardless of size, vary smoothly with temperature, pressure, and so forth; it's only in the so-called "thermodynamic limit" ( $L \rightarrow \infty$ ) that discontinuities or singularities can arise. <sup>13</sup>

As already noted, the total energy is not well defined in an infinite system, and so neither is the probability of a single infinite-volume spin configuration. How then does one define infinite-volume thermodynamic states? Not too surprisingly, this can be handled in a manner analogous to how we dealt with ground states. As before, there are two different but equivalent approaches.

The first focuses on *ratios* of probabilities for two infinite-volume spin configurations differing from each other by a finite set of spins. Any two such configurations differ by a finite energy  $\Delta \mathcal{H}$ , and so the ratio of their probabilities of appearance is proportional to  $\exp(-\beta \Delta \mathcal{H})$ .<sup>14</sup>

The second approach is to consider limits as  $L \to \infty$  of these probabilities on  $\Lambda_L$ —but not for individual spin configurations, whose probabilities tend to zero in this limit. Instead, one considers the probabilities of configurations specified by the values of any *fixed*, *finite* set of spins as  $L \to \infty$ . As in the ground state case, all possible sequences of boundary conditions must be considered: just as changing boundary conditions at zero temperature could change the ground state configuration in a fixed window, so a change in boundary conditions at *positive* temperature could change the *probability* of a given spin configuration in that window. A thermodynamic state is consequently generated for those sequences in which the probability of specific values for *any* fixed, finite set of spins settles down to a limit as  $L \to \infty$ .

Whichever approach one prefers leads to the same conclusion: at fixed  $\beta$ , infinite-volume thermodynamic states are probability measures on *all* infinite-volume spin configurations. <sup>15</sup> A given thermodynamic state  $\rho$  has a finite, well-defined energy per spin, free energy per spin, magnetization per spin, and so on, all of which can be calculated using the information it contains. These are examples of *global* quantities because they depend on *all* the spins. We are also interested in *local* quantities, such as *correlation functions*, which we now describe.

Consider the product of  $k \ge 1$  arbitrarily chosen Ising spins  $\sigma_{x_1}, \sigma_{x_2}, \ldots, \sigma_{x_k}$ ; in any *particular* spin configuration this product is either +1 or -1. However, a thermodynamic state  $\rho$  assigns a specific probability (call it p) for the set of all spin configurations for which this product equals +1, and another

probability (1 - p) for the set in which equals -1. Therefore, in the state  $\rho$  the expected value of the product, denoted  $\langle \sigma_{x_1} \sigma_{x_2} \dots \sigma_{x_k} \rangle_{\rho}$ , will be p(+1) + (1 - p)(-1) = 2p - 1.

This naturally leads to the possibility of *mixed* thermodynamic states, and corresponding mixtures of probability measures. Suppose that in the state  $\rho$  the two-point correlation function  $\langle \sigma_x \sigma_z \rangle_{\rho} = 0.2$  and in another state  $\rho'$  it's -0.4. One can then construct a third, *mixed* state, such as  $\rho'' = 0.3\rho + 0.7\rho'$ ; what this actually means is that

$$\langle \sigma_x \sigma_z \rangle_{\rho''} = 0.3 \langle \sigma_x \sigma_z \rangle_{\rho} + 0.7 \langle \sigma_x \sigma_z \rangle_{\rho'}$$
$$= 0.3(0.2) + (0.7)(-0.4) = -0.22, \quad (7.1)$$

and similarly for all other correlation functions. In general, if  $\rho$  and  $\rho'$  are distinct thermodynamic states, then so is  $W\rho + (1 - W)\rho'$  for any W between 0 and 1.

Hopefully, the mathematical meaning of a mixed state is clear; one just computes its correlation functions as in (7.1). But what does a mixed state *really* mean?

Suppose we go back to  $H_2O$  right at its boiling point,  $\beta_c$ . We'll choose  $\rho_l$  to be the state describing liquid water at its boiling temperature and  $\rho_v$  to be the state describing water vapor at that same temperature. For concreteness, we'll take  $\rho'' = 0.4\rho_l + 0.6\rho_v$ . If one samples configurations from the probability measure  $\rho_l$ , they would all look like liquid water: that is, they would all have the density and other properties of liquid water just as it's about to boil. Similarly, sampling from  $\rho_v$  would give configurations with the density and other properties of water vapor also at the boiling temperature. From this one might guess that  $0.4\rho_l + 0.6\rho_v$  would yield configurations with some properties of liquid and some properties of gas; but this is *not* what happens. Instead, if one samples many configurations randomly from  $\rho''$ , about

40% would look entirely liquidlike and the remaining 60% would look entirely vaporlike. You always find entirely one or the other.

Here's a somewhat tongue-in-cheek example of a mechanism by which such a mixed state could arise. Suppose you're a contestant in a popular American game show from the 1960s. The host shows you three closed, unmarked doors, and you must choose one to determine your prize. Behind one lies \$300 and behind the other two lies nothing. Your *expected* winnings are (1/3)\$300 + (2/3)\$0 = \$100, but you will go home with either \$300 or nothing at all.<sup>16</sup>

We noted in section 5.5 that the *physical* thermodynamic states are called pure states, but we've so far avoided saying precisely what they are, other than suggesting that they represent a specific phase of a substance such as liquid water or water vapor, as opposed to mixed states, which are statistical mixtures of distinct phases. We're now ready to be a bit more precise.

The short but perhaps not entirely satisfying definition is that a pure state  $\rho$  at a given temperature T is any infinite volume thermodynamic state that is *not* a mixture—that is,  $\rho$  cannot be expressed in the form  $W\rho_1 + (1 - W)\rho_2$  with 0 < W < 1 and with  $\rho_1$  and  $\rho_2$  distinct thermodynamic states (all at that same T, of course). This simply means that no matter what choice of W,  $\rho_1$ , and  $\rho_2$  you make, you can always find some finite set of spins  $x_1, x_2, \ldots, x_k$  such that

$$\langle \sigma_{x_1} \sigma_{x_2} \cdots \sigma_{x_k} \rangle_{\rho} \neq W \langle \sigma_{x_1} \sigma_{x_2} \cdots \sigma_{x_k} \rangle_{\rho_1} + (1 - W) \langle \sigma_{x_1} \sigma_{x_2} \cdots \sigma_{x_k} \rangle_{\rho_2}.$$
 (7.2)

Now, this negative way of defining a pure state  $\rho$  in terms of what its correlations do *not* do is probably less satisfying than having a positive definition. And there does exist such a positive

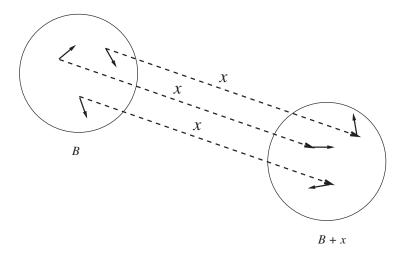


Figure 7.4. The spins in a particular set B consisting of three (non-Ising) spins and its translation B + x.

formulation, which says that a state  $\rho$  is pure if it satisfies certain correlation decay properties.

Using a more compact notation, let  $\sigma_A = \sigma_{x_1} \sigma_{x_2} \cdots \sigma_{x_k}$ , and let B denote another set of spins. Finally, let B + x denote a third set of spins, each of which is a distance x from its corresponding spin in B, as shown in figure 7.4.

Then  $\rho$  being pure means that for every A and B,

$$\langle \sigma_A \sigma_{B+x} \rangle_{\rho} - \langle \sigma_A \rangle_{\rho} \langle \sigma_{B+x} \rangle_{\rho} \to 0$$
 (7.3)

as  $|x| \to \infty$ . Roughly speaking, a pure state is one in which two random variables such as  $\sigma_A$  and  $\sigma_C$  have very small correlation if the regions A and C (which corresponds to B+x above) are very far apart.<sup>17</sup>

An important feature of infinite-volume thermodynamic states is that any state has a *unique* decomposition into pure states [29]. That is, a thermodynamic state  $\rho$  can be written in a unique way

as a sum (finite or infinite), 18

$$\rho = \sum_{i} W_{i} \rho_{i}, \tag{7.4}$$

where the  $\rho_i$ 's are pure states and the  $W_i$ 's—called the *weights* of the pure states in  $\rho$ —are non-negative and add up to one.<sup>19</sup> Equation (7.4) is both nontrivial and extremely important in what follows.<sup>20</sup>

If you find some of this discussion difficult to follow, that's all right. The take-home message is simply this: pure states are important because they underlie the thermodynamic structure of any macroscopic system, and moreover, if many pure states exist in the spin glass, that means there are many *distinct* spin glass phases, which would make them very exotic materials indeed.

We are now ready to tackle one of the central unresolved questions in spin glass theory: in the EA or similar realistic models in various finite dimensions, what does the low-temperature spin glass phase (if there is one) look like? In particular, what is the number of pure states? And if there are many, can a single large volume "hold" a thermodynamic state that is a nontrivial mixture of many pure states? These questions cut to the heart of the fundamental nature of spin glasses.

# 7.3 Scenarios for the Spin Glass Phase of the EA Model

Of course, the answer could be trivial: there could be no phase transition at all, and the spin glass could be a paramagnet all the way down to zero temperature. This is known to happen in one dimension and is believed (though still not proved) to be the case in two. It could also happen that there *is* a phase transition but no broken spin-flip symmetry. This could be the case if  $q_{EA} = 0$  (see equation (4.5)) at all nonzero temperatures,

but correlation functions for even numbers of spins change their behavior suddenly at some  $T_c$ .

The latter is an interesting possibility, but there's no evidence for it that we're aware of. On the other hand, there exists at least *some* evidence in favor of a phase transition with broken spin-flip symmetry in dimensions greater than (and possibly equal to) three [1,78–80, 235, 236]. So let's assume, as do most workers in the field, that in sufficiently high dimensions there is a phase transition at some dimension-dependent  $T_c(d)$ , and that the low-temperature phase is characterized by a nonzero  $q_{EA}$ . In that case, what should the low-temperature phase look like?

At a minimum there would have to be at least two pure states; just as with ground states, pure states would come in pairs. The members  $\alpha$  and  $\tilde{\alpha}$  of a pair would then be related by  $\langle \sigma_{x_1}\sigma_{x_2}\cdots\sigma_{x_k}\rangle_{\alpha}=\pm\langle \sigma_{x_1}\sigma_{x_2}\cdots\sigma_{x_k}\rangle_{\tilde{\alpha}}$ , where the plus sign corresponds to k even and the minus sign to k odd.

The question then becomes, how many *pairs* of pure states are present? And does the answer depend on *d*? And if there are many pairs, how are they related? Is the structure similar to what was found in the SK model?

There is much lively debate about the answers to these questions.<sup>21</sup> The various conjectures—and that's all they remain as of this writing, hence our usage of "scenarios" in describing them—correlate closely with the question of whether the EA model behaves in whole or in part like the SK model. We turn now to this question.

# 7.4 The Replica Symmetry Breaking and Droplet/Scaling Scenarios

Recall from section 5.6.1 that the spin overlap  $q_{\alpha\beta}$  plays an important role in describing the SK spin glass phase. The overlap

for the EA model is defined essentially as in (5.3), with  $\alpha$  and  $\beta$  now understood to be pure states. In short-range models, however, one needs to be careful: as in section 7.1, the use of windows is required, as follows.<sup>22</sup> For the usual cube  $\Lambda_L$ , consider a window of linear extent  $L_w$ , with  $L_w \ll L$ . One calculates the overlap as in (5.3), but using only the spins lying within the window. One then takes both  $L \to \infty$  and  $L_w \to \infty$ , with the constraint that  $L_w \ll L$  always. The reasons for doing this are discussed in [239]; the essential idea is that one wants to extract thermodynamic information only, eliminating spurious, nonuniversal effects that could arise from the boundaries.

As in the SK model, when  $\alpha = \beta$ ,  $q_{\alpha\alpha}$  is expected to be the same for all  $\alpha$  and to equal  $q_{EA}$ . Similarly,  $q_{\alpha\bar{\alpha}} = -q_{EA}$ .

Now, if the EA model behaves as suggested by the replica symmetry breaking analysis of the SK model, there should be many pure states and many overlap values  $q_{\alpha\beta}$  between  $-q_{EA}$  and  $+q_{EA}$ . Conjectures asserting that the broken symmetry structure of the EA model resembles that of the replica symmetry breaking analysis will be called *RSB scenarios*.

But scenarios have also been proposed asserting that the EA model behaves in a sharply different way from the SK model. The most important of these is the *droplet/scaling* scenario, introduced independently by McMillan [246], Bray and Moore [247, 248], and Fisher and Huse [249–252]. Droplet/scaling is based on a heuristic analysis of how the thermodynamic "cost" of flipping a large region (or droplet) of spins in a pure state depends on the spatial scale of the droplet. This analysis leads to the conclusion that the low-temperature spin glass phase comprises only a *single* pair,  $\alpha$  and  $\tilde{\alpha}$ , of pure states. As a consequence, boundary conditions (such as free or periodic) that give equal probabilities to any spin configuration  $\sigma$  and its flip  $-\sigma$  lead to a very simple mixed thermodynamic state  $\rho = (1/2)\alpha + (1/2)\tilde{\alpha}$ . This in turn means that the only overlaps are at  $+q_{EA}$  and  $-q_{EA}$ ,

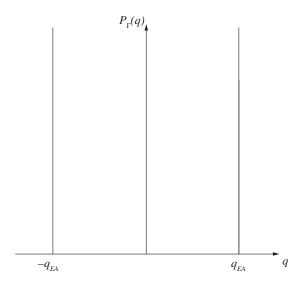


Figure 7.5. The overlap structure predicted by droplet/scaling. Here  $\Gamma$  refers to a general thermodynamic state, as discussed in section 7.9. This overlap structure is also predicted by chaotic pairs (section 7.10).

exactly as in figure 5.2, but with the pair of  $\delta$ -functions now at  $\pm q_{EA}$  (figure 7.5).

While this may seem rather dull compared to the RSB scenario (one sometimes hears the claim that droplet/scaling makes the spin glass "look like a ferromagnet"), it actually contains a few surprises of its own. One is that, just as the RSB scenario implies a richer, more complex structure of pure states than the ferromagnet, droplet/scaling predicts a much *simpler* structure: in fact, it doesn't look like a ferromagnet at all. Why is that?

Well, in addition to the simple uniform positively and negatively magnetized states, the Ising ferromagnet has other, non-translation-invariant pure states that can be generated through specially chosen boundary conditions (such as all boundary spins

equal to +1 on the top half of the volume and all equal to -1 on the bottom). These are states that have a "domain wall," separating up and down spins, running through the sample (for details, see [245]). So in fact the uniform ferromagnet has *many* pure states (in three and higher dimensions at low temperature), of which two are translation-invariant and infinitely many are not.<sup>23</sup> According to droplet/scaling, on the other hand, the spin glass has just two pure states, period, no matter how one chooses the boundary conditions, and regardless of whether this choice uses information about  $\mathcal J$  or not. Consequently, according to droplet/scaling the spin glass has *fewer* pure states than the ferromagnet.

The other surprise is that droplet/scaling asserts that this exceedingly simple pure state structure holds in all finite dimensions (above the lower critical dimension, which in this scenario lies between d=2 and d=3). That is, there is no upper critical dimension (section 5.1) above which mean field theory is correct, and not only at criticality, which would be surprising enough, but even in describing the low-temperature phase. Proplet/scaling asserts that the SK model is altogether pathological and cannot guide thinking about realistic spin glass models in any dimension and at any temperature—strong stuff, indeed. We'll explore reasons why this might be so a little later. Before doing that, though, we return to the RSB scenario and explore how its features might appear in the EA model.

# 7.5 The Parisi Overlap Distribution

Defining overlaps between pure states seems straightforward enough, but what happens when you have a mixed thermodynamic state and you try to compute overlaps? What you'll find is that your results won't be fixed but instead will fluctuate

randomly, with a probability distribution of possible values. This randomness is a direct consequence of the statistical nature of mixed states, as previously discussed. If you sample many spin configurations from  $\rho = (1/2)\alpha + (1/2)\tilde{\alpha}$ , then about half will look entirely like those from  $\alpha$  and the rest will look entirely like those from  $\tilde{\alpha}$ . So, if you continually and independently sample states from  $\rho$  and compute overlaps between successively chosen pairs, half the time you'll get  $q_{EA}$  and the other half  $-q_{EA}$ , as in figure 7.5.

In RSB scenarios life is even more complicated: here the relevant thermodynamic states are not mixtures of just two pure states but are weighted sums of many—in fact, infinitely many, just as in (7.4). So now what do things look like?

As previously described, a single spin configuration sampled from such a  $\rho$  will look entirely like one chosen from some particular one of the pure states  $\alpha_i$ , with probability  $W_i$ . Thus, the overlap distribution coming from such a  $\rho$  has probability  $W_iW_j$  for the value  $q_{\alpha_i\alpha_j}$ . Since all  $\alpha_i$ 's and  $\alpha_j$ 's with nonzero weights are possible, the overlap distribution  $P_\rho$  that arises from  $\rho$  is

$$P_{\rho}(q) = \sum_{i} \sum_{j} W_{i} W_{j} \delta(q - q_{\alpha_{i}\alpha_{j}}). \tag{7.5}$$

In RSB scenarios, infinitely many distinct overlap values have nonzero probabilities in this sum, although the bulk of the probability will be concentrated on some finite set of values.

As noted, the  $q_{\alpha_i\alpha_j}$ 's can be anywhere between  $-q_{EA}$  and  $q_{EA}$ , but the only way to get exactly  $q_{EA}$  is to have  $\alpha_j=\alpha_i$  and the only way to get  $-q_{EA}$  is to have  $\alpha_j=\tilde{\alpha}_i$  (or equivalently  $\alpha_i=\tilde{\alpha}_j$ ). The RSB scenarios, like the droplet/scaling scenario, will thus have nonzero probabilities for overlap values of  $\pm q_{EA}$ , but unlike droplet/scaling they will also have other values strictly between  $-q_{EA}$  and  $q_{EA}$ , as in figure 5.3 or 5.4.

To proceed in our description of the various RSB scenarios for the EA model, we need to review and extend our earlier discussion in section 5.6.2 about self-averaging and non-self-averaging in disordered systems.

### 7.6 Self-Averaging and Non-Self-Averaging

In a disordered system such as the EA spin glass, certain quantities will naturally depend on  $\mathcal{J}$ , the realization of all the couplings, with this dependence persisting even in the thermodynamic limit when the system size  $L \to \infty$ .

For example, consider the correlation  $\langle \sigma_x \sigma_y \rangle_{\alpha}$  for specific nearest-neighbor sites x and y in some pure state  $\alpha$  at a low temperature T (and thus large inverse temperature  $\beta$ ). Consider two spin configurations differing only in  $\sigma_x$ , with the first having  $\sigma_x = \sigma_y$  and the second  $\sigma_x = -\sigma_y$ . Then their ratio of probabilities will be proportional to  $\exp(-\beta \Delta \mathcal{H})$ , with  $\Delta \mathcal{H}$  as usual the energy difference between the two configurations. To make things simple, suppose  $J_{xy}$  happens to be very large and positive, while the other couplings connected to x are small; then it is not hard to see that the first configuration is far more likely to appear than the second. Since  $\langle \sigma_x \sigma_y \rangle_{\alpha}$  equals the probability in the pure state  $\alpha$  that  $\sigma_x = \sigma_y$  minus the probability that  $\sigma_x = -\sigma_y$ , it must be very close to +1 for any state  $\alpha$  at that temperature. Now, if we change  $\mathcal{J}$  so that  $J_{xy}$  is large in magnitude but negative in sign, then similar reasoning shows that  $\langle \sigma_x \sigma_y \rangle_{\alpha}$  must be close to -1. That is, a change in a single coupling of  $\mathcal{J}$  led to a large change in  $\langle \sigma_x \sigma_y \rangle_{\alpha}$ .

Thus we see that *local* quantities,  $^{26}$  in this case correlation functions, depend on  $\mathcal{J}$ . And the same is true for thermodynamic states in general since they are determined by all their local correlations. None of this is surprising. On the other hand, *global* 

quantities, such as the mean magnetization,

(1/Window Volume) 
$$\sum_{x} \langle \sigma_x \rangle_{\alpha}$$
, (7.6)

and the EA order parameter

(1/Window Volume) 
$$\sum_{x} (\langle \sigma_x \rangle_{\alpha})^2$$
, (7.7)

are expected (in the limit of large window volume) to depend neither on  $\mathcal J$  nor on  $\alpha$ ; as in the SK model, they are self-averaging.

All this is analogous to the classical statistical fact that a large number N of repeated but independent measurements of some quantity (e.g., the number obtained after averaging over many repeated rolls of a pair of dice) gives a sample average that approaches a fixed value—the theoretical population mean—as  $N \to \infty$ . This is so even though two different observers, doing two independent trials, will come up with quite different sequences of measured values.

Self-averaging is so common in statistics, probability theory, and more familiar areas of statistical physics that it came as something of a shock to learn that the RSB analysis of the SK model, as already discussed in section 5.6.2, predicts self-averaging only for  $q_{EA}$  but *not* for the full overlap distribution.

How does this translate to the EA model?

It turns out that there is not a unique way to transcribe concepts from the SK to the EA model. We will first describe the *standard* RSB scenario of the EA model, called that because it corresponds to most informal descriptions up to the mid-1990s. In this scenario there is a mixed thermodynamic state  $\rho_{\mathcal{J}}$  (the subscript denotes explicit dependence on the coupling realization) with a decomposition into pure states, as in (7.4), and overlap distribution, as in (7.5), such that all the quantities

appearing in these two decompositions are non-self-averaging (except as usual for  $q_{\alpha\alpha}=q_{EA}$  and  $q_{\alpha\bar{\alpha}}=-q_{EA}$ ). The non-self-averaging quantities, in addition to  $\rho_{\mathcal{J}}$  itself, include the pure states  $\alpha_i(\mathcal{J})$ , their respective weights  $W_i(\mathcal{J})$ , and the overlaps  $q_{\alpha_i(\mathcal{J})\alpha_j(\mathcal{J})}$ . In particular the overlap distribution  $P_{\rho_{\mathcal{J}}}$  should depend on  $\mathcal{J}$ , both where the  $q_{\alpha_i\alpha_j}$  overlaps are located in  $[-q_{EA}, q_{EA}]$  and their probability weights, as in figures 5.3 and 5.4.

Another feature of RSB, and hence of this scenario, is that when averaging  $P_{\rho_{\mathcal{J}}}$  over the  $\mathcal{J}$ 's to obtain P(q), the  $\delta$  function overlaps between  $-q_{EA}$  and  $q_{EA}$  are smoothed out to give a continuous distribution (figure 5.5)—except that  $\delta$  functions remain at  $\pm q_{EA}$ , since the  $q_{\alpha\alpha}$ 's (and  $q_{\alpha\alpha}$ 's) are self-averaging and do not depend on  $\mathcal{J}$ .

Can such a scenario for the EA model actually occur? We shall now see that it cannot.

## 7.7 Ruling Out the Standard RSB Scenario

The standard RSB scenario outlined in the previous section is summed up succintly in the quotation from [92] in section 5.4. It has the following features:

- 1. A mixed thermodynamic state  $\rho_{\mathcal{J}}$  that decomposes into an infinite sum of pure states.
- 2. An overlap distribution  $P_{\rho_{\mathcal{J}}}(q)$  that is an infinite sum of  $\delta$  functions, located both at the  $\mathcal{J}$ -independent values  $\pm q_{EA}$  and at many  $\mathcal{J}$ -dependent values  $q_{\alpha\beta}$  between  $-q_{EA}$  and  $+q_{EA}$ .
- 3. A  $\mathcal{J}$ -averaged overlap distribution P(q) whose only  $\delta$  functions appear at  $\pm q_{EA}$ .

It turns out, however, that any such scenario can be ruled out on mathematical grounds [253]. The key is that the EA model has a certain kind of translational symmetry that would be inherited by the state  $\rho_{\mathcal{J}}$ . The translational symmetry here is an extension to disordered systems of the type discussed in section 1.3.

Recall that in nondisordered systems, translational symmetry comes from the fact that the Hamiltonian  $\mathcal{H}$  is unchanged when all the spatial vectors  $\mathbf{r}_i$  are replaced by  $\mathbf{r}_i + \mathbf{c}$ , with  $\mathbf{c}$  an arbitrary constant vector. In the EA model, the  $\mathbf{r}_i$ 's are just the lattice locations where the spins reside and  $\mathbf{c}$  is restricted to be a lattice vector, just as when we looked at crystal symmetries. For a *fixed* typical  $\mathcal{J}$ , the EA Hamiltonian  $\mathcal{H}_{\mathcal{J}}$  does *not* have this type of translational symmetry since the  $J_{xy}$ 's very much do depend on x and y; if you move to the right by, say, five lattice constants you can easily observe a difference in your local environment.

But there still exists a more subtle kind of translational symmetry: the *probability distribution* of  $\mathcal{J}$  is unchanged by lattice translations because at all bonds  $\langle x,y\rangle$ , the corresponding coupling  $J_{xy}$  is independently chosen from the same distribution. This is the proper notion of translational symmetry for a disordered system, that is, a *statistical* translational symmetry. The result is a simple translational symmetry for the overlap distribution  $P_{\rho_{\mathcal{J}}}$ : when each  $\langle x,y\rangle$  is translated to  $\langle x+\mathbf{c},y+\mathbf{c}\rangle$ , the correspondingly translated  $\mathcal{J}$ , which we denote by  $\mathcal{J}+\mathbf{c}$ , gives an overlap distribution  $P_{\rho_{\mathcal{J}+\mathbf{c}}}$  that is *exactly the same* as  $P_{\rho_{\mathcal{J}}}$ . In plain(er) English, finite translations by  $\mathbf{c}$  have no effect, in the thermodynamic limit, on overlaps. Put another way, the calculation of the overlap distribution  $P_{\rho_{\mathcal{J}}}$  in an infinite system yields the same result no matter where you choose the origin.

So the overlap distribution  $P_{\rho_{\mathcal{J}}}$  is a function of  $\mathcal{J}$  but is unchanged under translations of  $\mathcal{J}$  to  $\mathcal{J}+\mathbf{c}$ . Fine, but so what? The so what is that because of the nature of the disorder distribution

of  $\mathcal{J}$ , with independent  $J_{xy}$ 's having identical distributions, it follows that  $P_{\rho_{\mathcal{J}}}$  must be self-averaging<sup>28</sup>—that is, it is the same for all  $\mathcal{J}$ 's<sup>29</sup> and equals its average P. Thus, properties 2 and 3 above are inconsistent with each other, and the standard RSB scenario cannot be valid.<sup>30</sup>

### 7.8 Chaotic Size Dependence and Metastates

Now, you may find this result somewhat disappointing. There's no question that RSB is a beautiful, even compelling scenario; might there not be other ways of adapting it to the EA model? If you're a diehard fan and want to find a modified RSB scenario for the EA model that cannot be ruled out so quickly, you would need to ask yourself, what property of the standard RSB scenario should you throw under the bus?

Almost certainly not statistical translational symmetry of  $(\rho_{\mathcal{J}}, \mathcal{J})$ , since that symmetry would be a consequence of using periodic boundary conditions.<sup>31</sup> And everyone in the spin glass community—theoretical physicists, computational physicists, and mathematicians alike—loves periodic. It's hard to find a more natural way to construct spin glass states.

But there is another property to consider, namely, that there is a *single* mixed state  $\rho_{\mathcal{J}}$  for each  $\mathcal{J}$  describing the  $L \to \infty$  limit of the EA model. This seems a little odd to discard, too; after all, if there are infinitely many pure state pairs, as RSB requires, can't they just be combined into a single mixed state? And if so, shouldn't that describe the thermodynamic structure of the spin glass?

The answer to the first is yes, but to the second, no. One *can* combine all the pure states into a single mixed state, but this state will then have self-averaging overlaps, as before. It might seem surprising that it is impossible to construct a single

mixed state whose overlaps are non-self-averaging, but one can prove [239, 255–257] that discarding the assumption of a single mixed state is the *only* way in which RSB can be rescued, and in a reasonably natural way. Doing so requires another mathematical tool, called the *metastate*. To understand the metastate, one first needs to be aware of a peculiar property of systems with quenched disorder called *chaotic size dependence* [258], which we now describe.

For a fixed low temperature T, let  $\rho_{\mathcal{J}}^L$  denote the periodic boundary condition thermodynamic state on the cube  $\Lambda_L$ . In homogeneous systems like ferromagnets, this just converges as  $L \to \infty$  to a mixed state, in the manner described in section 7.2. One might initially have expected something similar to occur in the spin glass. That, after all, is what would one expect convergence in general? That, after all, is what would be needed for a single  $\rho_{\mathcal{J}}$  to describe the large-L behavior of  $\rho_{\mathcal{J}}^L$ . But it was shown (in [258]) that, if many pure state pairs exist,  $\rho_{\mathcal{J}}^L$  may not settle down to a single  $\rho_{\mathcal{J}}$ . Instead, as L becomes increasingly large,  $\rho_{\mathcal{J}}^L$  may continually wander around, "sampling" from among all possible thermodynamic mixed states. These different mixed thermodynamic states are composed of different choices for the weights or different choices for the pure states (or both) that appear in the decomposition (7.4).

There is an interesting dynamical analogy to this. Many nonlinear dynamical systems display chaotic behavior; rather than settling down to a single fixed point, the system wanders forever on a fractal subset of dynamical state space known as a *strange attractor*. (For an introductory review, see [259].) In our context, the size L of the system replaces time, and the "trajectory" of the system, rather than a sequence of points in dynamical phase space, consists of the thermodynamic state "seen" in each  $\Lambda_L$ . This analogy led in [258] to the term *chaotic size dependence* (CSD) to describe this type of behavior.

If it occurs, CSD means that there would be many different limits of  $\rho_{\mathcal{J}}^{L_i}$ , along different choices of cube sizes  $(L_1, L_2, L_3, \ldots)$ , and in order to obtain convergence one would need to choose these  $L_i$ 's in a very special way, using the information contained in  $\mathcal{J}$  (we call this choosing the cube sizes in a  $\mathcal{J}$ -dependent way). On reflection, this behavior might seem quite plausible for a complex system like the EA model. But even if plausible, how could one describe such a complicated large-L behavior when a single limiting  $\rho_{\mathcal{J}}$  does not suffice? Again, reverting to English (more or less), how does one relate the thermodynamic  $(L \to \infty)$  behavior to that observed in large finite volumes? In homogeneous systems, this is straightforward; in disordered ones, much less so.

Dynamical systems theory provides a suggestion, namely, that when a system is sufficiently chaotic, its behavior for large time is described not by the state of the system itself at any particular time but instead by a *probability measure on the state space of the system*. This measure provides, roughly speaking, the fractions of time that the system asymptotically spends in different regions of its state space. That is, even though the system itself never settles down, with its representative point in dynamical state space forever wandering on a strange attractor, the amount of time it spends in each well-defined coarse-grained region *does* converge to a limit.

This type of approach was proposed for the EA model and other disordered systems [239, 255–257] in situations where CSD was known or suspected to occur, or where the possibility of its occurring had to be considered. In the EA model, the probability measure we need to deal with is one living on the space of all thermodynamic states (mixed as well as pure) for a fixed  $\mathcal{J}$  and temperature T. Such probability distributions were called *metastates* in [255], where they were first introduced in the EA setting, but they were also introduced earlier

(see [260]) in a different type of disordered system, known as a random field magnet (a uniform ferromagnet subject to a random external magnetic field). Just as thermodynamic states assign probabilities to different spin configurations, metastates assign probabilities to different thermodynamic states (which can be pure or mixed). Or more roughly, if there are many thermodynamic states, then different ones will appear in different subsets of volumes. The metastate then tells you the probability of seeing a particular thermodynamic state in an arbitrarily chosen volume.

#### 7.9 A New RSB Scenario

So, if you're not scared off by the prospect of dealing with metastates, then life gets interesting. Metastates can be used to provide an improved RSB scenario for the EA model, one that is not ruled out by the arguments in section 7.7. Whether this new scenario itself is free of internal contradictions is still not known, although arguments presented below indicate that it's not. Still, as of this writing it remains the only viable RSB scenario out there.

Let's use our understanding of the metastate to see how an RSB scenario might look in the EA context. Metastates replace the single  $\mathcal{J}$ -dependent overlap distribution  $P_{\rho_{\mathcal{J}}}$  by a *random*  $P_{\bar{\rho}_{\mathcal{J}}}$ .<sup>33</sup> As a random object, it has its own distribution, which we'll call  $\kappa_{\mathcal{J}}^{overlap}$  and which determines the probabilities of the various overlap distributions on  $[-q_{EA}, q_{EA}]$  corresponding to the different thermodynamic states.

Translating back into English (again), the thermodynamic mixed state  $\rho_{\mathcal{J}}^L$  varies chaotically as L changes. That means that in two arbitrarily chosen volumes one will typically see *different* 

mixed thermodynamic states. "Different" might mean a different collection of pure states, or the same pure states but with different weights, or some combination of the above.

So, instead of a single mixed thermodynamic state in the infinite-volume limit, we have to consider a collection of *infinitely many* different mixed thermodynamic states, each an infinite sum of pure states with specific weights—and therefore each with its own particular overlap distribution. Each of these thermodynamic states has a certain likelihood in the metastate, and therefore so does each corresponding overlap distribution. The likelihood of finding a particular overlap distribution in an arbitrarily chosen volume is determined by the quantity we call  $\kappa_{\mathcal{T}}^{overlap}$ .

Those of you still awake are probably asking yourself the following: Isn't this more complicated construct  $\kappa_{\mathcal{J}}^{overlap}$  still subject to the same translation-invariance properties as before? And then doesn't that rule out non-self-averaging by the same arguments?

In fact, you're right about the first part:  $\kappa_{\mathcal{J}}^{overlap}$  is translation-invariant; it is unchanged under the translation  $\mathcal{J} \to \mathcal{J} + \mathbf{c}$  and so is indeed self-averaging. But the fact that its nature is so different from  $P_{\rho_{\mathcal{J}}}$ , the overlap distribution arising from a single mixed state, leads to an entirely different picture—one that can survive our earlier arguments.

A key way to see how is to focus on the notion of dispersal of the metastate  $\kappa_{\mathcal{J}}$  and of the corresponding  $\kappa_{\mathcal{J}}^{overlap}$ . By dispersal of  $\kappa_{\mathcal{J}}$  we simply mean that it does not assign all of its probability to a single thermodynamic state  $\rho_{\mathcal{J}}$ ; that is,  $\kappa_{\mathcal{J}}(\Gamma)$ , where  $\Gamma$  denotes any possible thermodynamic state, is not of the form  $\delta(\Gamma-\rho_{\mathcal{J}})$ . Nondispersal is what happens when  $\rho_{\mathcal{J}}^{L}$  settles down to a single limit  $\rho_{\mathcal{J}}$  as  $L\to\infty$ —essentially, the old way of looking at things. Indeed, that is so in the droplet/scaling scenario, where  $\rho_{\mathcal{J}}$  is of the form  $(1/2)\alpha+(1/2)\tilde{\alpha}$ . It's also

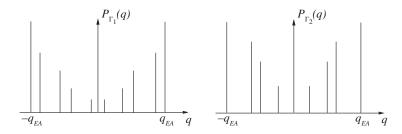


Figure 7.6. Two different overlap distributions corresponding to different thermodynamic states, as might arise in the same window within two different volumes, but with the same coupling realization  $\mathcal{J}$ , in the nonstandard RSB scenario.

what happens in the standard RSB scenario except that there  $\rho_{\mathcal{J}}$  decomposes into many pure states, as in (7.4).

Nondispersal of thermodynamic states  $\kappa_{\mathcal{J}}$  in turn implies nondispersal of overlap distributions as determined by  $\kappa_{\mathcal{J}}^{overlap}$ ; all probability is assigned to the single overlap distribution  $P_{\rho_{\mathcal{J}}}(q)$ . In droplet/scaling, this is  $(1/2)\delta(q-q_{EA})+(1/2)\delta(q+q_{EA})$ , while in standard RSB it is as in (7.5).

The nonstandard aspect of the RSB scenario we are now introducing replaces—or, if you like, reinterprets—non-self-averaging by dispersal. The "distribution of overlap distributions" is indeed self-averaging; it is the same for every  $\mathcal{J}$ . But as the volume varies, the overlap distribution now varies with it. As before,  $\Gamma$  denotes a given mixed thermodynamic state, which in RSB consists of an infinite sum of pure states with specific weights, as in (7.4). Now, in our new and improved RSB scenario, the thermodynamics comprises an *infinite* set of such mixed  $\Gamma$ 's. Different volumes can correspond to different  $\Gamma$ 's (as before, we'll stick with using periodic boundary conditions on all volumes), and therefore the observed overlap distribution will also vary with the volume (figure 7.6).

So, we've replaced the  $\mathcal J$  dependence of a quantity like  $P_{\rho_{\mathcal J}}(q)$  with the  $\Gamma$  dependence of  $P_{\Gamma}(q)$  as  $\Gamma$  is sampled from  $\kappa_{\mathcal J}(\Gamma)$ . Likewise, instead of averaging over the disorder distribution of  $\mathcal J$  to obtain the averaged overlap distribution P(q), we instead average over  $\Gamma$  (or equivalently, over volumes) for any fixed  $\mathcal J$ :

$$P(q) = \int P_{\Gamma}(q) d\kappa_{\mathcal{J}}(\Gamma) = \int P'(q) d\kappa_{\mathcal{J}}^{overlap}(P').$$
 (7.8)

We'll get the same result, independent of the  $\mathcal{J}$  we've chosen: it should look like figure 5.5.

Summarizing, the nonstandard RSB scenario has the following features:

- 1. A dispersed metastate  $\kappa_{\mathcal{J}}(\Gamma)$  on mixed thermodynamic states  $\Gamma$ , each of which decomposes as an infinite sum of pure states.
- 2. The overlap distribution  $P_{\Gamma}(q)$  for any  $\Gamma$  sampled from  $\kappa_{\mathcal{J}}$  is an infinite sum of  $\delta$  functions, located both at  $\pm q_{EA}$  and at many  $\Gamma$ -dependent values between  $-q_{EA}$  and  $+q_{EA}$ . Now, overlap distributions such as appear in the two parts of figure 7.6 correspond to overlaps measured in *different volumes but the same*  $\mathcal{J}$ , rather than different  $\mathcal{J}$ 's.
- 3. A  $\Gamma$ -averaged overlap distribution P(q) whose  $\delta$  functions are only at  $\pm q_{EA}$ . This is done for fixed  $\mathcal{J}$  and is the same for every  $\mathcal{J}$ , and looks like figure 5.5.
- 4. If ultrametricity occurs, it can only occur *separately* within each individual  $\Gamma$  (or volume). It cannot hold for *all* the pure states, taken together, in the metastate.

So, translational symmetry does still have consequences—namely, that  $\kappa_{\mathcal{J}}^{overlap}(P')$  does not actually depend on  $\mathcal{J}$ . But that is not a death blow anymore, because we've reinterpreted non-self-averaging: according to feature 2 above,  $\kappa_{\mathcal{J}}^{overlap}(P')$  is

well dispersed, with the  $\delta$  function locations of P' moving around as P' varies (corresponding to  $\Gamma$  varying in the dispersed metastate  $\kappa_{\mathcal{J}}(\Gamma)$ ), and so there is no longer an obvious contradiction between features 2 and 3.

So, while this looks considerably different from the original RSB perspective, it retains the maximal amount of "RSB-ness" that the EA model can sustain. But does it actually *occur*?

At the time of this writing, it has not been rigorously ruled out. Numerical evidence has been provided both for and against it. (There are too many papers to list here, but see, e.g., [261–263] (for) and [264,265] (against).) There are also some rigorous results that strongly suggest that nonstandard RSB *cannot* occur in realistic spin glass models. One is a result on invariance of the metastate with respect to changes of boundary conditions [239].

This invariance is a new kind of symmetry altogether. Suppose we replace periodic boundary conditions in the finite cube  $\Lambda_L$  by antiperiodic boundary conditions, where spin values on opposite faces of the cube are the negatives of each other rather than the same. It turns out that the metastate and all of its properties are the same, regardless of whether one uses periodic boundary conditions for all L, all antiperiodic, or any arbitrary choice of periodic and antiperiodic. Similarly, the metastate is the same for any sequence of fixed boundary conditions used, and so on. This insensitivity to boundary conditions is fundamentally at odds with heuristic expectations of how any RSB or otherwise complicated mixed-state scenario should behave in short-range models<sup>34</sup>; it strongly suggests a simple mixed state and overlap structure. A second piece of evidence is a recent result [267] that the behaviors of the SK and EA models are fundamentally different when one perturbs the couplings; it's difficult to see how the same type of low-temperature ordering in both models can be consistent with this result.

## 7.10 Two More (Relatively) New Scenarios

Let's review what we have so far.

Instead of thinking about a single mixed thermodynamic state as describing spin glass behavior, we *may* need to think about an entire probability distribution, denoted  $\kappa_{\mathcal{J}}(\Gamma)$ , over many mixed thermodynamic states  $\Gamma$ . Furthermore, each  $\Gamma$  has its own overlap distribution  $P_{\Gamma}(q)$ ; the probability distribution of these  $P_{\Gamma}(q)$ 's is given by  $\kappa_{\ell}^{overlap}(P)$ .

Combining this with our original introduction of metastates by analogy with chaotic dynamical systems leads to the following picture of what's going on. As L gets large, the finite-volume state  $\rho_{\mathcal{J}}^L$  looks like a state  $\Gamma$  sampled from  $\kappa_{\mathcal{J}}$ , and the overlap distribution obtained from  $\rho_{\mathcal{J}}^L$  looks like one sampled from  $\kappa_{\mathcal{J}}^{overlap}$ . In this spirit, the nondispersal of both  $\kappa_{\mathcal{J}}$  and  $\kappa_{\mathcal{J}}^{overlap}$  in the droplet/scaling scenario means that for an increasing sequence of very large L's, the  $\rho_{\mathcal{J}}^L$ 's will have settled down to look like one fixed thermodynamic state and the overlaps that will be seen will be close to  $+q_{EA}$  about half the time and close to  $-q_{EA}$  the other half. This can be described as a settled-down state and a simple (boring?) overlap as  $L \to \infty$ .

On the other hand, the dispersed nature of both  $\kappa_{\mathcal{J}}$  and  $\kappa_{\mathcal{J}}^{overlap}$  in the nonstandard RSB scenario means that as  $L \to \infty$ , the states are chaotic and the overlap distribution is constantly varying.

RSB and droplet/scaling are the two most-studied spin glass scenarios, but what about other possibilities? It turns out that the metastate picture naturally leads to other scenarios that are just as plausible (and are backed by neither more nor less evidence) as RSB or droplet/scaling. For example, couldn't it happen that  $\kappa_{\mathcal{J}}$  is dispersed but  $\kappa_{\mathcal{J}}^{overlap}$  is not? Of course it could. In fact, it's rather a sensible picture. In this scenario, every  $\Gamma$  sampled from  $\kappa_{\mathcal{J}}$  is of the form  $(1/2)\alpha + (1/2)\tilde{\alpha}$ —but not with one single

pure state pair  $\alpha$ ,  $\tilde{\alpha}$  for *all* samples, rather with a *different*  $\alpha$ ,  $\tilde{\alpha}$  for *each*  $\Gamma$ .

This would mean that, for a typical large L, the finite-volume state  $\rho_{\mathcal{I}}^{L}$  looks like it does in droplet/scaling: an equal-weight mixture of a pure state and its flip. But unlike droplet/scaling, the pure state pair  $(\alpha_L, \tilde{\alpha}_L)$  does not settle down but rather varies chaotically as  $L \to \infty$ . In other words, there are *infinitely* many pure state pairs, and consequently infinitely many mixed thermodynamic states  $\Gamma$ . But, because now each  $\Gamma$  is just a simple mixture of a pure state and its global flip, the overlap  $P_{\Gamma}(q)$  is independent of  $\Gamma$ . When you measure the overlap in a window in any large finite volume, it unvaryingly looks like figure 7.5:  $P_{\Gamma}(q) = (1/2)\delta(q - q_{EA}) + (1/2)\delta(q + q_{EA})$ , even though the pure state pair appearing in a fixed window continues to change chaotically with L. In this scenario, the states are chaotic but the overlaps are boring. This scenario has been called the *chaotic pairs* model and was introduced in [255] (with a brief foreshadowing in [258]).

Regardless of whether this scenario holds, there are two important conclusions to be drawn from it. The first is that the overlap structure is not necessarily a good indicator of whether there are few or many pure states. Chaotic pairs is an infinite-state picture with a simple overlap structure. Overlaps are simply too coarse and global a tool to determine the number of pure states [268], which themselves are very much locally determined objects [269] (recall the discussion in section 7.6).

The second conclusion is that there are *many* possible infinite-state scenarios, of which RSB is only one. By the same token, droplet/scaling is but one of many possible *two*-state pictures (of which we'll see another in a moment). While RSB *predicts* many pure states and droplet/scaling predicts only a single pair, each makes many other predictions as well. For example, RSB has a lot to say about the detailed relationships among the pure states and

their overall thermodynamic structure, and these are markedly different from the predictions of chaotic pairs. Moreover, the scenarios we've presented all make different predictions about the nature of low-energy excitations above the ground state(s), about interface structures and energies between different ground or pure states, and other low-temperature properties.

The moral is, many-states alone is not synonymous with RSB, nor is a single-pair scenario synonymous with droplet/scaling.

One final scenario, commonly denoted the "TNT" picture [270, 271],<sup>35</sup> has generated considerable interest. This scenario, supported by some numerical simulations (but see also [272]), proposes that in the EA model at low temperatures, low-lying excitations have a nontrivial spin overlap with the ground state but a trivial "edge" overlap  $e_{\alpha\beta}$ , where

$$e_{\alpha\beta} = (1/\text{Window Volume}) \sum_{\langle x,y \rangle} \langle \sigma_x \sigma_y \rangle_{\alpha} \langle \sigma_x \sigma_y \rangle_{\beta}.$$
 (7.9)

So, for example, the spin overlap between a ground state  $\alpha$  and its spin-reversed partner  $\tilde{\alpha}$  is -1 but its edge overlap is +1. The edge overlap provides information on the interface density between two states: the higher the density, the smaller  $e_{\alpha\beta}$ . In the TNT picture, the interface density is not zero in finite volumes, but its dimensionality is smaller than that of the lattice. Consequently, the interface density  $\rightarrow$  0 and  $e_{\alpha\beta} \rightarrow$  1 as (Window Volume)  $\rightarrow \infty$ .

This excitation structure is different from that of RSB, droplet/scaling, or chaotic pairs. So TNT is indeed a new scenario, but is it a two-state or a many-state picture? It turns out that it can be either [273].<sup>36</sup> However, it does not fit quite as easily into a many-state picture as a two-state, so if something like TNT turns out to be correct, we suspect that the low-temperature spin glass phase would consist of a single pair of pure states.

# 7.11 Why Should the SK Model Behave Differently from the EA Model?

What is it about spin glasses—and more generally, systems with quenched disorder and frustration—that makes them behave so differently from more conventional systems? Of course, it depends on which difference you're talking about, and in previous chapters we've noticed many differences in both thermodynamic and dynamical behavior. In this section we'll narrow our focus considerably, concentrating on a single question.

Recall that in conventional systems, such as ferromagnets, mean field theory provides an excellent guide to low-temperature behavior—the nature of the broken symmetry, the type of order parameter—and even correctly describes the critical behavior near the phase transition above an upper critical dimension. So if it's true that the low-temperature behavior of the SK model does not describe that of the EA model in *any* finite dimension—and this remains an unresolved issue—what is it about these models that could make them behave so differently?

Consider again the SK Hamiltonian (5.1), and note that the typical coupling strength scales as  $N^{-1/2}$ , where N is the number of spins. This means that the "effective coupling" between two spins  $\sigma_i$  and  $\sigma_j$  depends on the size of the system:  $J_{ij}^{\text{eff}} = J_{ij}/\sqrt{N}$ . There are N(N-1)/2 of these couplings, and they completely determine the spin configuration energies, and therefore the state structure for this N-spin system.

Next, suppose we look at a much larger M-spin system,  $M \gg N$ , that includes the smaller N-spin system, as shown in figure 7.7.

Now the original N(N-1)/2 couplings have been greatly reduced in magnitude, while a much larger number of new couplings (M(M-1)/2 - N(N-1)/2) have entered the picture. While all couplings equally determine the spin configuration

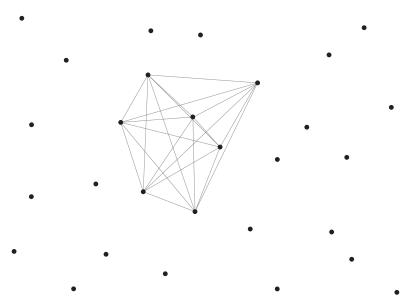


Figure 7.7. A system of M=29 sites. Within that system is a subsystem of N=7 sites, with the N(N-1)/2=21 couplings shown explicitly. The total number of couplings in the entire system is M(M-1)/2=406 (couplings touching sites outside the original N-spin system are not shown). The central point is that in the original 7-spin system, the typical coupling strength is order  $1/\sqrt{7}$ ; in the larger 29-spin system, the strength of each of those same original 21 couplings has decreased to  $1/\sqrt{29}$ . As  $M\to\infty$ , the strength of those original 21 couplings goes to zero, and their influence on the configuration of the original 7 spins vanishes.

energies, the effect of the original N(N-1)/2 couplings has become much smaller, as they become overwhelmed by a much larger set of new couplings. As  $M \to \infty$ , the effect of the original couplings (along with their magnitudes) becomes vanishingly small. As a result, the earlier "pure state structure" corresponding to the original N-spin system is completely washed out.

But isn't this true for all infinite-range models, whether homogeneous or disordered? Yes, but the difference is that the couplings in disordered systems are *statistically independent*, while those in homogeneous systems are not. So, in the infinite-range ferromagnet, even though the coupling strength decreases like 1/N, the couplings all have the same sign and so "reinforce" each other: the pure state structure doesn't really change as the number of spins increases.

For disordered systems, on the other hand, the signs and magnitudes of the couplings in the smaller *N*-spin system are *independent* of the added couplings in the larger *M*-spin system. The result is that *any fixed, finite set of couplings will eventually have a negligible effect on the spin glass state when the number of spins becomes large enough.<sup>37</sup> It's the combination of the physical couplings scaling to zero in the SK model and their statistical independence<sup>38</sup> that presumably lies at the heart of the problem [275].* 

In contrast, short-range models do not share this peculiar feature: the couplings outside a particular fixed, finite region can act at most on the boundaries of the region. How strong an effect this presents is presently unknown. In principle, the EA model in sufficiently high dimensions *could* share the thermodynamic behavior of the SK model, but arguments like the one presented above, along with the results discussed in section 7.9, make this seem doubtful.

## 7.12 Summary: Where Do We Stand?

We've presented four different scenarios for the low-temperature spin glass phase in the EA model, assuming there's a phase transition leading to broken spin-flip symmetry: RSB, droplet/scaling, chaotic pairs, and TNT (in chronological order of appearance).<sup>39</sup> Which of these (if any) actually holds?

We don't know. Numerical evidence has been garnered for all pictures; analytical or rigorous evidence is growing but incomplete. We've noted that standard RSB can be rigorously ruled out, and there's some evidence that nonstandard RSB can't hold either. But the jury's still out.

Can we at least say something about numbers of ground or pure state pairs? Unfortunately, not much. There are interesting models that allow one to compute numbers of *ground* states [277–279], but they're unrealistic and probably not much of a guide for what's going on in the EA model. Some headway has recently been made in *two* dimensions, including a proof that only a single pair of ground states appears in the *half* -plane [244]. Numerical evidence has been provided that the ground state structure in three dimensions is similarly trivial [242, 280], but that's disputed by others [272, 281–283]. The upshot is, we just don't know. And we're basically nowhere in answering the question of numbers of *pure* states at nonzero temperature. 40

Still, although the big questions—existence of a phase transition the number and structure of ground and pure states, the nature of broken symmetry in the short-range spin glass—remain at large, a significant amount of analytical progress has nonetheless been made. A number of new phenomena have been discovered (some of which are found in both the SK and EA models), including chaotic size dependence and others not mentioned (or glancingly mentioned), such as temperature and disorder chaos [285] and stochastic stability [286]; new mathematical machinery, such as metastates, has been developed; and the thermodynamic behavior of short-range spin glasses, regardless of whether it resembles that of the SK model, has been shown to be rich, subtle, and multi-layered.

And now we'll close by looking back over where we've been and asking whether spin glasses deserve the label "complex system."

## 8

## ARE SPIN GLASSES COMPLEX SYSTEMS?

We conclude our primer with a brief consideration of how spin glass science fits into the larger area of complexity studies. As putative complex systems, spin glasses are unusual in that they fall neatly into standard, well-defined disciplinary categories: condensed matter physics and statistical mechanics. That concepts and techniques arising from their study served usefully in other disciplines was initially an unanticipated bonus. Be that as it may, these applications have come to define the field as much as its original, narrower domain. The fact that a significant number of nonphysicists and nonmathematicians are even aware of spin glasses, regardless of whether they know what they are, indisputably owes to this wider impact.

The question remains whether spin glasses can justifiably be called "complex systems," even in the absence of a universally agreed-upon definition of complexity. The answer seems to grow less clear over time. Spin glasses have long sat outside the mainstream of much of modern complexity research (which we'll

take, for lack of a better guideline, to be those studies that emerge from centers and institutes with the words "complexity" or "complex systems" somewhere in their names), which has largely focused on adaptive systems, networks, games and cooperation, and similar areas.

Nevertheless, we assert below that spin glasses still merit the title of "complex systems." Our assertion follows not only from current treatments of the subject but also from an older and still valid tradition that laid the basis for much of the modern study of complexity. In this chapter we discuss briefly what we consider to be three of the foundational papers of complexity studies,<sup>2</sup> and how we envision spin glasses as fitting into the general vision that emerges from these papers. We also take a brief look at how they relate to more modern views of complexity. And finally, we'll close with a discussion about how recent studies of spin glasses, especially of short-range models, might affect older notions of how spin glasses contribute to our understanding of complex systems.

## 8.1 Three Foundational Papers

#### 8.1.1 Warren Weaver and the Birth of Complexity Science

In 1947, Warren Weaver [287] delivered an address remarkable for its prescience and broad historical sweep. While predicting an imminent transition of scientific momentum from physics to biology, which turned out true enough, the paper goes much deeper. Noting two developments, one technological and the other social, arising from the recent war, Weaver predicted that in combination, the two would fundamentally transform the nature of science. The technological advance was, of course, the advent of the modern electronic computer; the social advance

was the formation of interdisciplinary teams to attack largescale problems, the Manhattan Project being the most famous example.

Weaver's main thesis was that together, these two would do more than make previously inaccessible problems tractable; they would alter altogether the type and nature of the problems that science considered.

In asking what role science should have in humanity's development, Weaver first looked back on the tremendous progress in the physical sciences since the time of Galileo, Kepler, and Newton. That progress was made possible by focusing on "problems of simplicity." This was not intended to mean that the problems themselves were simple. Weaver's point was rather that, through inspired physical intuition, an overwhelming mass of irrelevant detail and inconsequential complication could be discarded, resulting in a situation in which a very small number of variables remained relevant in elucidating the system's fundamental nature.<sup>3</sup>

As Weaver pointed out, problems of this kind cannot readily be found in the life sciences, resulting in the fact that, as of the mid-twentieth century, they remained largely descriptive in character rather than quantitative or analytical.

Weaver next turned to another, more recently developed, foundation of science, which focused on "problems of disorganized complexity." Here one looks at the other extreme, where the number of independent variables (e.g., position and momentum of atoms in a gas) becomes enormous. Progress is possible because one does not need to know, even in principle, the individual behavior or laws governing an individual degree of freedom. All that matters is the presence of a high degree of randomness, so that statistical methods can be employed to analyze average system properties. Owing to the huge number of random variables, this collective behavior becomes predictable (and sometimes even orderly).

Obvious examples include not only the thermal disorder (section 5.1) of a collection of atoms or spins at high temperature but also the motion of stars in a galaxy, the usefulness of actuarial tables, the laws of heredity and population genetics, and the profitability of casinos.

Between them, these two approaches can handle an enormous variety of scientific questions. But there remained an as yet (in 1947) largely untouched "great middle region," where the "problems of organized complexity" reside. These are problems with an intermediate to large number of variables, but neither simplification to a few relevant variables nor the statistical methods used in disorganized complexity can gain traction. These problems all exhibit "a sizable number of factors which are interrelated into an organic whole." They include problems of gene expression, protein folding, economic behavior, sustainability of societies: essentially the set of questions whose answers can alter the course of human events for better or worse. A couple of generations later these came to be called, simply, problems of complexity.

These problems, and many others from the biological, physical, psychological, and social sciences, do not yield to traditional mathematical techniques. Because of the interrelatedness of their many variables, they cannot be reduced to few-variable model systems. And the statistical techniques that worked so well for problems of disorganized complexity are ineffective in dealing with organized complexity: their variables are too interdependent and correlated. At the time of Weaver's writing, they were largely intractable problems.

Weaver's inescapable conclusion was that science must be poised to make its "third great advance." He argued that the tools were at hand to carry this program forward—as noted, the advent of electronic computing and the interdisciplinary team approach that was so effective in solving problems that a small group of individuals could not have tackled alone.

Weaver's paper was written decades before spin glasses emerged on the scene. How do they fit into his schema? One might take a step back and ask the same question about systems in an ordered state, such as crystals or ferromagnets. On the face of it, they don't fit neatly into either category, and yet they were also well understood by the time of Weaver's paper. But ordered condensed matter takes some elements from each category. Zero-temperature properties can be deduced through quantum mechanics, using translation symmetries as a necessary simplifying tool. What about low but nonzero temperatures? The advent, a decade or two later, of concepts such as broken symmetry and the order parameter did in fact reduce the number of variables needed to describe the ordered state. With these powerful concepts, the statistical methods used to understand disorganized complexity could then be brought to bear.

Spin glasses, on the other hand, challenge this program. They can't be simplified through a perturbative analysis around a ferromagnetic state. They don't exhibit disorganized complexity; paramagnets do. But they don't appear to be an example of organized complexity either.

Nevertheless, they do share some features with the latter. They can't be solved by the old methods, at least not without new concepts; they exhibit a number of interesting emergent properties, such as hierarchical organization of overlaps (see in particular the next section); and they transcend disciplinary boundaries, in the sense described in chapter 6. Perhaps they could be thought of as a bridge between simple systems and disorganized complexity, on the one hand, and organized complexity on the other. We'll encounter this idea again below.

But let's return to Weaver's paper, written before spin glasses came along. His argument may seem obvious today, particularly because things evolved almost exactly as Weaver had predicted. But science then was still heavily disciplinary, with some exceptions here and there, and so his address generated little resonance at the time and was largely ignored, or more likely forgotten, for close to half a century. Intellectually, though, it set the stage for other thinkers, coming from different backgrounds and with varying agendas, to expound on the inevitability of a new wave of science and what it might look like. We turn to one of these next.

#### 8.1.2 Herbert Simon and the Architecture of Complexity

Herb Simon was an economist, political scientist, sociologist, and psychologist, who made seminal contributions not only to all those fields but also helped establish the modern research areas of artificial intelligence, information processing, and decision-making theory. In this section we discuss his influential 1962 paper proposing hierarchical organization as a fundamental principle underlying the architecture of complex systems [102, 103].

Simon's wide-ranging interests, comprising organization theory, general systems theory, and information and communication theory, among many others, led him naturally to a general consideration of complex systems (a term he may have picked up from Weaver's paper, which he cites, emphasizing that he shall be concerned solely with "organized complexity"). Then as now, a formal definition of complexity was lacking, and Simon kept it simple and general:<sup>4</sup> a complex system is "one made up of a large number of parts that interact in a nonsimple way." Almost as a tangential thought, he struck what must have been at the time a controversial position: that such systems are essentially nonreductionist in that a knowledge of their elementary constituents and the laws governing their interactions may not be sufficient to deduce their collective properties as a whole. This theme is expounded in much greater detail in Anderson's paper "More Is Different" [288], to be discussed in the next section.

Simon considered both static and dynamic properties of complex systems, but the unifying theme of his paper is that a central feature of complex systems is their hierarchical structure: a complex system comprises interacting subsystems, each of which likewise comprises subsubsystems, and so on until, after at least several such levels, one reaches a lowest, elementary set of components. Interactions within subsystems are much stronger than those between subsystems, leading to a "near-decomposability" that can be modeled mathematically. Simon emphasizes that there exist some universal features—which can be found in a variety of biological, physical, and social systems—of this hierarchical architecture; as such, it can serve as a unifying concept of complexity theory.

Simon makes a compelling case, probably familiar to most readers in one form or another, that building a hierarchical structure provides a plausible scenario of how complexity can evolve. But his introduction and formalization of the idea of a nearly decomposable system are arguably the paper's most novel contributions. Consider again the ultrametric structure of figure 14. One might, for example, interpret the nodes at the bottom level as thermodynamic states. The shorter the ultrametric distance, the greater the overlap. One could then construct an "overlap matrix"5 that looks like the one on the following page, with  $q_{EA}>q_1>q_2>q_3>q_4$ . The basic structure of a nearly decomposable matrix is displayed here: a block diagonal structure with off-diagonal subblocks, with the larger-magnitude matrix elements (representing stronger interactions or faster transition rates, and so on) residing within the blocks and smallermagnitude elements, representing weaker interactions, residing between the blocks.<sup>6</sup> In a nearly decomposable matrix, the offdiagonal elements should be nonzero but very small, so unless  $q_1 \ll q_{EA}$ , the matrix above doesn't quite fit the bill. The point, however, is that the *structure* of the matrix is essentially the same.

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Of course, Simon had in mind more dramatic examples of complex systems than spin glasses (which weren't even identified as such for more than a decade after he wrote his paper). But it's of some interest that a nearly decomposable matrix structure emerges in a natural and unanticipated way from the structureless SK Hamiltonian.

#### 8.1.3 Philip Anderson and "More Is Different"

Phil Anderson's 1972 article "More Is Different" [288] brings us full circle back to the centrality of the notion of broken symmetry, but with something of a twist. The article intended to discredit what Anderson called the "constructionist" hypothesis: the notion that "fundamental science" consisted primarily in the discovery of new laws at the microscopic level. Anderson distinguished this from reductionism, rooted in the hierarchical

structure of science. The meaning of "hierarchy" in this context is somewhat different from Herb Simon's; here it simply captures the incontrovertible fact that atoms and molecules obey the underlying laws of elementary particle physics, that solid state physics and chemistry obey the underlying laws of atomic and molecular physics, biology obeys the laws of chemistry, psychology those of biology, and so on.<sup>7</sup>

The fallacy that Anderson argues against is the seductive corollary that, once one has hold of the fundamental laws, the rest is extrapolation and application.<sup>8</sup> In particular, he notes that the constructionist hypothesis breaks down in going from one level to another because of "the twin difficulties of scale and complexity." (Interestingly, the term "complexity" rarely appears, although its presence permeates the paper.) Although it may be true that "the elementary entities of science X obey the laws of science Y," it is nevertheless *not* the case that "science X is 'just applied Y'":

At each stage entirely new laws, concepts, and generalizations are necessary, requiring inspiration and creativity to just as great a degree as the previous one. Psychology is not applied biology, nor is biology applied chemistry.

Where is the evidence for this assertion? Anderson's central argument is that it lies in the pervasive presence of broken symmetry<sup>9</sup> in both condensed matter and particle physics.<sup>10</sup>

Much of the rest of the paper is devoted to explaining the concept of broken symmetry and its centrality in understanding condensed matter. We have already discussed all this at length in chapter 1. Where things get interesting is the extension of these ideas to what we would today call complexity science. The flow of the argument connects, whether consciously or not, with Weaver's, but with the added unifying notion of broken symmetry (not yet formulated at the time Weaver wrote his paper).

Anderson proposes that broken symmetry notions might be extendable to systems that are not only regular, like ordinary crystals or ferromagnets, but also contain information—DNA and proteins being the obvious examples. However, in analyzing biological systems one needs to consider symmetries in time rather than space. It is reasonable, though of course speculative, to suppose that broken temporal symmetry could be useful in understanding both information processing and dynamical phenomena in living systems.

What is not speculative, however, is that only three years later the EA order parameter [74], which manifestly focuses on the temporal rather than spatial domain, was proposed. This is interesting. It suggests (returning to the speculative mode) that spin glasses might be an intermediate step between the rather rigid broken spatial symmetry of the crystal and the more fluid, noninert broken symmetries that could be present in more functional, information-carrying structures, such as those found in living organisms.<sup>11</sup>

In any case, the punch line is the enormously pleasing suggestion that "at some point we have to stop talking about decreasing symmetry and start calling it increasing complication."

By which, of course, he means complexity.

### 8.2 Spin Glasses as a Bridge to Somewhere

By 1984, the Parisi solution of the SK model had been worked out (nonrigorously) and interpreted; the application of spin glass concepts to biology, computer science, and elsewhere had become a minor industry; and, most significant, talk of complexity and complex systems was in the air. Late that year, two meetings that were to become the founding workshops of the Santa Fe Institute took place, bringing together physicists, mathematicians, chemists, biologists, computer scientists, and a variety of

social scientists. Their talks were gathered by David Pines into a collection called *Emerging Syntheses in Science* [289]; the first research article in that collection, by Phil Anderson, touted spin glasses as "a bridge between biology, statistical mechanics, and computer science" [290].

For those readers who've stayed the course, the narrative of Anderson's article is by now familiar. Spin glasses are governed by a very large number of variables, are characterized by quenched randomness and frustration, and possess a rugged free energy landscape with many minima (both thermodynamic and metastable states in the SK model, and at least metastable states in the EA model). These features enable them to lend themselves naturally to a variety of problems in computer science and biology. The former include new analytical methods for optimization problems and new algorithms (simulated annealing, Hopfield-type neural computation). The latter include applications to neural science, evolution, protein dynamics, and the immune response.

At the time those meetings were held, this was all new and powerful stuff. The question remains, how well did it hold up, and how might we think of spin glasses within the framework of complexity today?

#### 8.3 Modern Viewpoints on Complexity

Before turning to this question, we take a brief look at the evolution of complexity science since the early 1980s. While a great deal has been written on the subject—a comprehensive treatment would be next to impossible to achieve in a full-length book, much less in a few paragraphs—in some ways we're still at square one. Not only is there no generally accepted definition of complexity; there are no universal guidelines for characterizing

a complex system, and no well-defined general principles for organizing our thinking. The field, in short, remains scientifically amorphous (in our opinion).<sup>12</sup> But this does not imply an absence of interesting and potentially important proposals.

#### 8.3.1 Measures of Complexity

As one might expect, much effort has gone into attempts to define appropriate measures of complexity; after all, constructing a successful measure would be tantamount to defining complexity. It would play the same foundational role as, say, Boltzmann's formulation of entropy in the nineteenth century played for the new science of thermodynamics.

Complexity measures proposed to date often focus in one way or another on information: how much a system contains, the history leading to its present information content, or its capacity for generating more information in the future. One of the earliest and still most useful measures of information content is due to Shannon [217],<sup>13</sup> who described a way to measure the information content encoded in a string of bits. And indeed, we saw in section 6.4.1 how spin glass modeling could demonstrate how large information content, in Shannon's sense, might arise in the prebiotic evolution of macromolecules. In some sense, the more "unpredictable" a given string is, the higher its Shannon information entropy (as it's called).

But there are many other ways to think about information. The well-known algorithmic complexity of Solomonoff, Kolmogorov, and Chaitin [291–294] defines the complexity of a string of bits in terms of its inherent randomness, that is, the size of the minimal program (as usual, on a universal computer) needed to produce the string as output. Think of a nonrandom sequence of N bits, such as 01010101011..., or the first N

digits of  $\pi$ . Both can be generated by algorithms that are much shorter than the strings themselves (for N large): these sequences are *compressible*. If, on the other hand, a description of an N-bit string cannot be generated from an algorithm much smaller than N bits itself, the string is incompressible, and has a high algorithmic complexity. It is clear that this is really a measure of randomness, not of complexity, and so is not immediately relevant; however, it serves as an important historical springboard for later developments.

Most measures of complexity attempt to quantify, in one way or another, the *difficulty* of constructing a complex system. To this end, Bennett [295, 296] introduced the notion of "logical depth." Briefly, this considers the computational *time* of the minimal program needed to produce a given output. "Thermodynamic depth," introduced by Lloyd and Pagels [297], attempts to distinguish between a system's randomness and its complexity by relating its entropy to all possible historical paths that can lead to its present state. In both these measures, the information content of a system is deeply entwined with its history; the more difficult it is to "build" a system, the greater its complexity. <sup>14</sup> Although neither of these proposals is the last word on the subject, their emphasis on a system's history—or set of possible histories—is satisfying and should almost certainly be an ingredient of an ultimately successful theory.

Other measures focus attention on actual structures. The "effective complexity" introduced by Murray Gell-Mann [299] stresses the importance of the structural regularities of a system, as opposed to its random, nonessential features. How does one separate the essential from the inessential? Admittedly, performing such a categorization is subjective, and it may be difficult or impossible to carry this program out perfectly for a given system. Nevertheless, one might be able to get a handle on the problem by "embedding the entity in question in a set of entities sharing the

regularities and differing only in other respects" [299]—in some sense, by considering the system in question as part of a larger universality class.

The last measure we discuss is the "statistical complexity" of Grassberger [300] and Crutchfield and Young [301]. Like some of the others, this approach attempts to remedy algorithmic complexity's assigning high complexity to random, as opposed to meaningful, strings of data. To do this, Grassberger and Crutchfield and Young focus on the *predictive* capabilities of a given subsequence of a data string. That is, one now directly attempts to extract a measure of "meaning," or at least usefulness, from a string of bits, by determining the causal "impact," so to speak, of a given sequence of bits on future sequences. Note that here, "future" can also refer simply to sequences of bits farther along the string. After all, the dynamical history of a putative complex system can be mapped onto such a string, and one can in principle study conditional probabilities of future subsequences given earlier ones.

We emphasize again that this very brief survey does not attempt to include all proposals but is intended instead to give a flavor of current thinking on the problem of defining a complexity measure (for a more comprehensive overview, see [302]). None has gained universal acceptance, and all are difficult to use, particularly in precisely defining some or most of their ingredient quantities. <sup>15</sup> Nevertheless, these attempts are useful in helping to guide our thinking in what we actually mean by a complex system.

As an aside, it is interesting to note that the basis for all of these proposals lies either in computer science or thermodynamics (in some cases, both). This may confine their usefulness to physical and computational systems; it remains difficult to see how to apply any in a quantifiable way to biological or social systems. Going further out on a limb, one might wonder whether a new

science of complexity should really be derivative from physics (through thermodynamics) or computer science.

But it's probably best at this point to allow the reader to form his or her own conclusions.

#### 8.3.2 General Features of Complexity

While these proposed measures all present interesting ways of thinking about complexity, it may be more useful to look for common strands that have proved robust over the years. Which features of putative complex systems repeatedly appear in treatments and discussions of the subject?

Many of these were presented back in the introduction and have recurred throughout the book. They include a capacity for adaptive behavior; the formation of structures (often with multiple scales) in space or time; a balance between rigid order and chaos; the ability to store, evolve, and transmit information; and a hierarchical or modular architecture. A system is more likely to display these features if it contains nonlinearity and feedback in its dynamics, quenched disorder in its thermodynamics, and multiple dynamically or thermodynamically stable states or outcomes. However, we still don't know whether any of these ingredients is strictly necessary, and they're almost certainly not sufficient in themselves.

In a real sense, complexity carries with it with an element of surprise; as pointed out by Goldenfeld and Kadanoff [303], complexity becomes manifest both when simple rules lead to complex structures and when complicated systems show simple regularities. In the former case, cellular automata and fluid behavior provide standard examples; in the latter, climate comes readily to mind. While the emergence of the unexpected is certainly not a sufficient condition for complexity—after all, it

happens all the time in science, and more generally in life—it's hard to imagine that it's not necessary. In this regard, it's fair to say that spin glasses have acquitted themselves well.

## 8.4 Spin Glasses: Old, New, and Quasi-Complexity

Throughout this book, we have encountered a good deal of evidence supporting the claim that spin glasses exhibit a number of features associated with complex systems. <sup>16</sup> First and foremost, they are inherently disordered: the dirt cannot be swept away by analyzing a spin glass through a perturbation about a "clean" or ordered system. The disorder *is* the essence of the problem. This is of fundamental importance, because in one form or another, it's a property that must be shared by all complex systems. Strict homogeneity or rigid ordering in a system would preclude any chance of its evolving.

Moreover, spin glasses exhibit frustration; in fact, they gave rise to a precise definition and mathematical analysis of the idea. The presence of conflicting constraints seems to receive less mention in the complexity literature than other properties, such as nonlinearity, hierarchical organization, striking a balance between rigid ordering and chaos, and the rest of the usual suspects. But it shouldn't. Without frustration, it's difficult to see how anything approaching complexity—with its generation, storage, and transmission of large information content—could arise. <sup>17</sup>

As we've seen, spin glasses have a rugged free energy landscape in state space with many optimal or near-optimal "solutions." These correspond to both metastable states and possibly, at least in high dimensions, to pure thermodynamic states. At the very least, they do have many thermodynamic states in their infiniterange version. And possessing multiple solutions, or dynamical outcomes, or steady states is a hallmark of all complex systems.

Moreover, the infinite-range version of the spin glass—the SK model—contains numerous other novel features: an exotic sort of symmetry breaking that cannot be quantified in terms of the microscopic properties of a single state, non-self-averaging, and an ultrametric structure of overlaps. The last, arising spontaneously from an essentially featureless Hamiltonian, displays features similar to Simon's nearly decomposable systems.

Perhaps most important, spin glass notions have served (and continue to serve) as a foundation for studying problems in fields as diverse as computer science and biology. They have given rise to new algorithms, new methods for solving graph-theoretic problems, and new ways of thinking about evolution and adaptation, protein dynamics, protein folding, neural networks, and a host of other problems that we haven't even mentioned. This transdisciplinarity is a crucial element of any problem purporting to relate to complex systems.

It's important to add that we've mentioned only *static* features of spin glasses. Because we've tried, with limited success, to keep this book as brief as possible, we've largely ignored (with the exception of section 4.3) the rich *dynamical* structure of spin glasses, which also exhibits important features usually associated with complexity. These include slow relaxation, irreversibility, history dependence, memory effects, and aging. If one is interested in directly applying complexity measures such as logical or thermodynamic depth to spin glasses, their nonequilibrium dynamical evolution may provide a fertile ground for exploration.

Now most of this, aside from its distillation into one place, is old news, well established by the late 1980s. We might therefore call it "old complexity." Which raises the question, in what sense can we look at advances in spin glass research over the last two decades to see whether seeds of a "new complexity" might have arisen?

At first glance, this program doesn't look promising. Much of modern complexity research deals with adaptive systems, whether biological, social, economic, or other. Although spin glass research has provided mathematical models useful in studying adaptation, spin glasses themselves don't adapt. As noted in the introduction, they really don't do much of anything—at least, compared to an organism, a social network, or a society.

So if there's a case to be made at all for a "new complexity," we'll have to look elsewhere. Perhaps this isn't necessary; old complexity may be perfectly sufficient as is. But it's worthwhile exploring whether anything lies beyond.

One place to search may be back at the roots of spin glass research, in the field of statistical mechanics. From time to time some workers have speculated that this old, well-established field may need to be revamped, or even fundamentally rethought, to accommodate spin glasses, not to mention their even more troublesome cousins, ordinary glasses. We believe that research since the early 1990s indicates that this view is too extreme. Nevertheless, as we've learned more, we've come to understand that it's necessary at least to rethink some older notions and deeply held assumptions.

There are several reasons supporting this view. One is the presence of chaotic size dependence and its usefulness for probing the existence of many thermodynamic states (section 7.8). More generally, new mathematical tools and notions, including the metastate (section 7.8) and stochastic stability (section 7.12), both created to study systems with quenched disorder, have already been shown to have a wide degree of applicability and the potential to lead to new ways of thinking about the statistical mechanics of inhomogeneous systems.

Besides providing new tools, spin glass research has enabled us to probe further and deeper into parts of statistical mechanics. Replica symmetry breaking—the broken symmetric structure of the SK model—helped overturn old assumptions and led to new ways of thinking about broken symmetry. But its presence in realistic spin glass models is controversial (section 7.12). If it is indeed absent there, where does that leave things?

Well, perhaps that would make things even more interesting. In classical statistical mechanics, mean-field theory has generally been an invaluable guide to low-temperature behavior, in particular the nature of a system's broken symmetry and corresponding order parameter. Mean field theory's primary drawback (section 5.1) is its inability to handle critical behavior close to  $T_c$ , because it neglects fluctuations. But even in conventional systems, there is an upper critical dimension above which mean field behavior sets in at  $T_c$ . If it turns out to be the case that mean field theory fails to provide an accurate description of the low-temperature spin glass phase in *any* finite dimension [238, 239, 249,250,253,255,256,268], then we really have something new and remarkable.<sup>19</sup>

Another fundamental core assumption of statistical mechanics challenged by spin glasses is the expectation that the thermodynamic limit reveals the bulk properties of large finite systems. In homogeneous systems this expectation is satisfied, and extrapolation between infinite and large finite volumes is straightforward. However, if above some dimension the spin glass phase turns out to possess many incongruent pure state pairs, <sup>20</sup> then the connection between the thermodynamic limit and the behavior of finite macroscopic systems becomes more subtle.

How so? As noted in section 7.8, the presence of many competing pure states leads to chaotic size dependence and necessitates use of the metastate. For an ordered system, the dynamical systems analog to the thermodynamic limit is a simple fixed point, and the thermodynamic state appearing in a large volume would be analogous to a point within the fixed point's basin of attraction, approaching the fixed point as  $L \to \infty$ .

In this case the two—that is, the thermodynamic state in a large volume and that described by the thermodynamic limit—look much the same. For a disordered system with many competing states, however, the relation between the thermodynamic limit and a particular large volume is analogous to that between a strange attractor and a single point wandering endlessly on an orbit approaching the attractor. This is a very different sort of relationship.

The possible divergence in behavior between short-range spin glasses in any finite dimension and infinite-range spin glasses may carry important lessons not only for statistical mechanics but also for complexity more generally; it may indicate the fundamental limits of the applicability of analogies between different types of systems. Complexity science thrives on analogy, and relies heavily on the transference of concepts and techniques from one field to another. Indeed, that has been a recurring theme throughout this book, and we're all for it. But there could well be limits to this program; perhaps at some point every complex system displays unique features at a fundamental level that are truly sui generis. If so, the concept of universality classes one of the central, unifying ideas of statistical mechanicsmay not be well-suited for the study of complex systems. In spin glasses, the possibly wildly different behaviors between short-range and infinite-range spin glasses—where one would have expected similar low-temperature ordering-could be a foreshadowing of the breakdown of universality<sup>21</sup> in the study of complexity. But drawing any conclusions at this point would be premature.

Are these and other potentially deep properties of spin glasses indicative of a new type of complexity? We'll have to leave that question open for the time being and allow each reader to judge for her- or himself. But looking back over the journey we've taken, we propose that spin glasses deserve at least the rubric

of quasi-complex system. Whether truly complex or not, they have provided mathematical descriptions of important aspects of complexity, and so in some respects have achieved the sort of bridge that Warren Weaver envisioned long ago.

This may well be one of the most remarkable—and surprising—features of spin glasses with regard to complexity: no one disputes that a truly complex system must be out of equilibrium, yet the study of *equilibrium* spin glasses has generated a host of deep mathematical structures that characterize complex systems more generally. It has provided a mathematical framework to sharpen and analyze the notion of frustration; shown quantitatively how organization, structure, and hierarchies can arise from blind randomness; and generated new models for the spontaneous generation of information. And while spin glasses may not be adaptive themselves, they've given rise to new mathematical descriptions of adaptation.

While much complex systems research remains descriptive or dependent purely on numerical simulation, spin glasses have, starting from a very compact and simple-looking energy function, yielded a cornucopia of new physical and mathematical results, tools, and concepts that can be applied to problems in biology, computer science, and elsewhere. And it's safe to assume that more are coming. So we'll gamble and speculate that spin glasses are truly deserving of being included in the roll call of complex systems—whatever that ultimately turns out to be.

# NOTES

#### Preface

- 1. Recognizing the terms is probably sufficient.
- 2. For those interested in these more comprehensive—but also technical—treatments, our recommendations include [1–10]. A nontechnical overview appears in [11]. A very recent book that appeared after this book went to press is *Perspectives on Spin Glasses*, by Pierluigi Contucci and Cristian Giardinà (Cambridge University Press, 2012).
- 3. Some will be only vaguely or intuitively defined, to be sharpened in later chapters.

#### Introduction

- 1. We'll assume the naming of the problem requires no further explanation.
- 2. Or was, originally. But no more. TSP-solving algorithms have since found numerous applications, such as constructing genome maps; see, for example, [12].
- 3. There are too many books on the general subject of complexity and complex systems for us to be able to provide a comprehensive list.

For those interested in learning more about the subject(s), there are many places to turn. There are, of course, the other books in this primer series, as well as the many books published under the Santa Fe Institute Studies in the Sciences of Complexity series. We list here a handful of others that the reader might enjoy: [14–20].

- 1. Some references for the interested reader include [13, 23–25].
- 2. So far we've discussed only examples of *global* transformations in which every particle undergoes the exact same transformation. There are also *local* (or *gauge*) transformations in which every particle undergoes its own *individual* change. An example might be every particle rotating about an internal axis but through an angle that can vary from particle to particle. The distinction between local and global transformations is important but not needed for the level of discussion here.
- Remember, this is only a *theoretical* exercise. The idea is to see whether such a transformation makes an observable difference. No one is talking about time actually running backward in the physical world.
- 4. Called a *boost*, this type of transformation plays a central role in relativity theory.
- 5. Phase transformations are important in quantum mechanics, which uses a wavelike description to describe matter.
- 6. A variable in boldface implies a vector quantity; otherwise the variable refers to a scalar.
- 7. As opposed to, say, speed or direction of travel.
- 8. We generally use primed quantities to denote variables after the transformation and unprimed quantities to denote the original variables.
- 9. Of course, they depend *indirectly* on *t* because the particle *positions* can change with time, but we care only about explicit, not implicit, dependences.

- 10. The system Lagrangian, for you mathematicians and physicists out there. While we're on a technical aside, we should note that the theorem applies only to *continuous* symmetries, that is, those that can be characterized by one or more continuous parameters.
- 11. By "long," we mean compared to the forces between atoms that hold the crystal together, which typically extend only about  $10^{-8}\,\mathrm{cm}$ .
- 12. This is a classical, as opposed to quantum mechanical, description, which is suitable for our purposes here.
- 13. Both  $\mathbf{p}_i$  and  $\mathbf{r}_i$  are functions of time, but to keep the notation simple we won't explicitly display that dependence.
- 14. We assume that the crystal is otherwise isolated and not subject to external gravitational, electrical, or other fields.
- 15. This assumes the atom can be treated as a pointlike particle, with no internal structure. In the case of argon this is a very good approximation.
- 16. Aside from greater density, slower speeds, and some short-range correlations in the liquid state, the basic picture at the atomic level looks much the same for the gas and the liquid.
- 17. Of course, on any realistic timescale, a given liquid or gas can actually assume an infinitesimal fraction of all available configurations. The point is that, by assumption, all are a priori equally probable.
- 18. This illustration is only for conceptual purposes, but in fact pictures such as this are commonly used in both particle and condensed matter physics to illustrate symmetry breaking. See [23–25] if you're interested in learning more.
- 19. Although any individual outcome breaks the symmetry, notice that if you look at *all* possible outcomes and combine them you restore the original symmetry, because all final resting places are equally likely.
- 20. Of course, a shift of one full lattice constant *R* returns an infinite crystal to the original state, and is considered to be the same outcome.
- 21. Again, as a technical aside, such excitations result from the breaking of *continuous* symmetries.

- 22. The basic ideas underlying the Higgs particle—central to modern particle physics—arose from applications of broken symmetry to superconductivity, central to modern condensed matter physics. The kind of broken symmetry in these cases is local rather than global.
- 23. Which in turn is related to the generalized rigidity that we referred to in the introduction.
- 24. The shape of the potential depends on temperature, and the circle where the potential is minimum moves out from the origin as temperature is lowered.
- 25. We hope it's clear that the word "phase" is used here in a completely different context from "phases of matter."
- 26. There are some niceties here we're skipping over. For example, to construct such a function we need to do some coarse-graining in which we divide space into subregions roughly the size of atoms or slightly larger.
- 27. With advance apologies to all of the great scientists who developed and continue to advance this deep subject. We only hope their aim is poor.
- 28. For those with knowledge of statistical mechanics, we're confining our discussion to the canonical ensemble.
- 29. Recall that in our recurring example of *N* argon atoms in three dimensions, a configuration is an enumeration of all 6*N* positions and momenta.
- 30. For a nice discussion of how this formula arises, see Feynman's book [27].
- 31. If you're not familiar with Boltzmann's constant  $k_B = 1.4 \times 10^{-23} J/^{\circ} K$ , it's sufficient to think of it simply as a conversion factor between temperature in degrees Kelvin (°K) and energy in joules (J), where  $1 J = 1 \text{ kg} \cdot \text{m}^2/\text{sec}^2$ .
- 32. By "appear," we mean the following. Mathematically, we're talking about an imagined collection—or *ensemble*—of identical systems at some fixed time. Each such sample system will contain a specific configuration whose probability of appearing in that system is determined by its energy according to the Boltzmann

distribution. Physically, this is supposed to correspond to following a single system through time, measuring its energy at, say, picosecond intervals as it continually assumes different microscopic configurations. If the system is in equilibrium at temperature T, then after many measurements the resulting energy histogram will follow the Boltzmann distribution. This assumes the presence of a deep property known as *ergodicity*, which remains unproved for most systems. For more information, see [27–29].

- 33. The term "thermodynamic state" refers to the collection of a huge number of microscopic configurations that are available to the system at a given temperature. We'll make this notion more precise later, but this is sufficient for the moment.
- 34. Because the force F and the potential V(x) are related through F = -dV/dx. Alternatively, you can just think of the system as a ball rolling downhill in V(x).
- 35. To keep the discussion brief and accessible, we're glossing over the facts that there are numerous types of crystals and that the simple cubic structure implied here is an oversimplification.
- 36. A good analogy is flipping a biased coin, say one that comes up heads with probability 2/3 and tails with probability 1/3. Of all possible sequences of N flips, the one with highest probability is the "ordered" configuration (representing the crystal) with all heads—but this occurs with the vanishingly small (if *N* is large) probability  $(2/3)^N$ . Instead, what you're overwhelmingly likely to see is a "disordered" sequence with roughly 2/3 heads and 1/3 tails. Any particular sequence of heads and tails is extremely improbable. But there are very many sequences with roughly 2/3 heads and 1/3 tails, and they overwhelm in number those with almost all heads. So we'll almost certainly end up seeing one of those disordered sequences, given that we don't generally care about the exact order in which heads and tails appear. Now you may be wondering, isn't it even more likely to see a sequence with roughly half heads and half tails, since there is an even greater (in fact, much, much greater) number of those? It's a good question, but the answer is no, it's not.

Even though there are indeed many more sequences with roughly half heads and half tails than any other ratio, the bias in the coin makes the probability of each of these sufficiently small that in the end, one is most likely to see roughly 2/3 heads and 1/3 tails in a typical sequence. It's the balance between the likelihood of a sequence with a certain head-to-tail ratio and the total number of such sequences that determines the most likely outcome of an actual trial.

- 37. Called the *Helmholtz* free energy.
- 38. The balance between the likelihood of a sequence and the number of similar sequences in the biased coin example is analogous to the competition between energy and entropy captured by the Helmholtz free energy.
- 39. We've noted earlier that these very same concepts have also been used extensively in particle physics, and have been essential in arriving at the highly successful synthesis known as the *standard model*. To learn more, see [25].
- 40. Which is one reason why the continual appearances of statements declaring the "end" of any field inevitably come to their own untimely ends.

- 1. As a consequence, the notion of equilibrium is intimately tied to the timescale of observation. On the scale of minutes, a glass of water can have unchanging temperature and volume, but over the course of hours, its volume changes noticeably owing to evaporation. The idea of equilibrium cannot be separated from notions of the measurement timescale, how strongly or weakly the system interacts with its external environment, and a host of other complications. A detailed treatment can be found in [28]; here we'll leave you with a delightfully succinct statement, due (of course) to Richard Feynman: "Equilibrium is when all of the fast things have happened, and all of the slow things have not."
- 2. The size of the entropy jump at crystallization is directly proportional to the heat released (absorbed) upon freezing (melting).

- More generally, although entropy cannot be directly measured, it can be inferred from specific heat measurements.
- 3. How quick is "sufficiently quickly" depends on the material in question. It can be as slow as a few degrees per hour (o-terphenyl in vacuum) or as fast as millions of degrees per second (many metals).
- 4. There are a number of theories and explanations as to why this happens, some very ingenious, but so far none that has achieved universal acceptance. A good review of the glass transition that also discusses various theoretical proposals appears in [31]; see also [32–34].
- 5. Yes, it's still in a sort of equilibrium, though in what's often called a *metastable* equilibrium.
- 6. There are some theories that assert that one is nevertheless hiding somewhere.
- 7. The word "quench" is used today in a wide variety of scientific and engineering contexts, of which this is only one. Its use in physics arose from metallurgy, where it referred to plunging a metal alloy (often steel) at very high temperature into a cold liquid. This rapid, nonequilibrium cooling preserved mechanical properties that might be lost under slow cooling that allowed equilibration along the way. The latter is referred to as *annealing*, which we'll meet again in chapter 6.
- 8. There are numerous general treatments of the modern approach to crystalline solids at an advanced undergraduate level; two of the most widely used are [37, 38].
- 9. From time to time, ideas based on localization have found their way into spin glass research; see, for example, [39–44].

1. Thorough discussions of the material covered in this chapter can be found in almost any undergraduate-level solid state physics textbook. Suggestions include [37, 38, 45, 46].

- 2. For an entertaining first-hand account of the discovery of spin, see http://www.lorentz.leidenuniv.nl/history/spin/goudsmit.html.
- 3. Of course, in addition to its intrinsic, or spin, angular momentum, the electron can have a nonintrinsic *orbital* angular momentum, and the latter *can* be changed, although in quantized steps. Unlike its spin, an electron's orbital angular momentum depends on its motion, and can be zero or as large as you like. The *s*, *p*, *d*, and *f* atomic orbitals familiar to students of chemistry and physics refer to the electron's orbital angular momentum state within the atom.
- 4. The reasons for this lie in quantum mechanics, which (as you may have noticed) we're skirting as gingerly as possible.
- 5. This is the basic principle behind the compass; the compass needle is a permanent magnet that can freely rotate, and it aligns itself with the earth's magnetic field.
- The motion of the spin as it tries to align with the field is more complicated than simply lining up, but this is not important for the discussion.
- 7. Notice that we've now reverted to that sloppy terminology where we use "spins" in place of "magnetic moments."
- 8. How high varies from solid to solid, but in all cases still well below the melting point.
- 9. Since the electron spin is attached to its host atom, and the crystal structure is maintained, the spin's position **x** stays more or less put, though it gets jostled a bit too. The important thing to remember is that the *orientation* of the spin is constantly changing, not its location.
- 10. For the remainder of this chapter, we will assume that magnetic moments behave like classical three-dimensional vectors, able to point equally well in any direction. This is actually never true at the atomic level, but in a variety of magnetic materials it works reasonably well as an approximation on a larger scale, where "spin" can refer to a coarse-grained average over many atomic magnets.
- 11. This is actually the *static* susceptibility, measuring the response to a static external field. There is also the *dynamic* susceptibility,

- which describes how well the system's magnetization follows an alternating external field.
- 12. A little thought should convince you that, while the ferromagnetic ground state accommodates itself easily to any sort of lattice, the antiferromagnetic one is more troublesome. What happens, for example, if we try to put the antiferromagnetic ground state onto a triangular lattice? We'll address this issue in section 4.6, where we take up the idea of *frustration*.
- 13. In honor of Louis Néel, who won the 1970 Nobel Prize in Physics for his work on antiferromagnetism (among other things).
- 14. Try to construct one using figure 3.3 as a guide. Remember that the order parameter should be a function of all of the spins that is zero in the high-temperature, or paramagnetic, phase and nonzero in the antiferromagnetic phase.
- 15. As noted earlier, this is not true for real atomic magnetic moments in crystals, but for some materials it's approximately true on a more coarse-grained scale.
- 16. Two of the founders of modern quantum mechanics.
- 17. But one thing we can note right away is that the summation over nearest neighbors means that the coupling between spins that are *not* nearest neighbors is zero. This is an idealization; more accurately, one expects the interaction strength between spins to fall off as the distance between them grows. For many solids this falloff is fast enough that the "nearest-neighbor only" approximation provides accurate results.
- 18. As noted earlier, this may be an average of thousands of individual atomic magnetic moments—which would still occupy a tiny enough region of the solid that we can simply think of it as a single magnetic moment at a well-defined point **x**.
- 19. In fact, the Hamiltonian (3.4) is called a *phenomenological* Hamiltonian: it doesn't purport to replicate the microscopic physics in detail but instead lumps together a great deal of complicated physics into a relatively simple form. The idea—or sometimes hope—is that a mathematical analysis of this relatively

simple-looking Hamiltonian will reproduce to reasonable accuracy the complicated physics of the real system.

- 1. Along with a number of widespread misperceptions about what is and isn't known.
- 2. An interesting personal take by someone present at the creation can be found in a series of short pieces by Philip Anderson in *Physics Today* [52–58].
- 3. Probably idiosyncratic.
- 4. Or more accurately, a related quantity called the *resistivity* to electrical conduction that depends on the material alone and not on the geometric properties of the wire.
- When they remain localized on the impurity atoms. Sometimes solid state effects cause the moments to vanish altogether, but we'll focus only on alloys where this doesn't occur.
- In fact, spin glass behavior usually persists at much lower concentrations, but one has to go to correspondingly very low temperatures to observe it.
- 7. At higher concentrations—roughly 10% or more—the placement of the impurity atoms becomes more regular than at low concentrations, and one ends up with an ordinary ferro- or antiferromagnet.
- 8. But if you're a physicist and are curious, the observations were of the onset of hyperfine splitting observed in Mössbauer studies [1].
- 9. Of course, this is also the case in both the ferromagnet and the antiferromagnet.
- Susceptibility data can be dynamic or static, depending on whether
  measurements are made with a static magnetic field or one oscillating at a fixed frequency.
- 11. This result itself is often taken as an indication that during the relaxation process, the system surmounts several successive barriers on a rugged free energy landscape, of the kind shown in figure 4.7. This picture is not needed for the present discussion, but we

- mention it here as an aside in anticipation of future discussions in section 4.9 and especially section 6.3.1.
- 12. Even more interesting behaviors, such as "rejuvenation," occur when the temperature is not held fixed during the course of the experiment.
- 13. More precisely, what is found is that, after a fast initial decay, the long-time system response can be expressed as a function that roughly scales with  $t/t_w$ .
- 14. However, there are materials, such as lithium holmium yttrium fluoride (interesting not only for spin glass physics but also for quantum entanglement and computing), in which such direct interactions *do* play an important role [72]. For recent work, see [73].
- 15. Meaning that the random variables are chosen from a continuum of values, in contrast to a *discrete* distribution such as  $\pm J$ . In the Gaussian case, the domain of each random variable is  $(-\infty, \infty)$ .
- 16. A probability distribution in which the continuous random variable  $J_{xy}$  is distributed according to  $P(J_{xy}) = \frac{1}{\sigma\sqrt{2\pi}}e^{-(J_{xy}-\mu)^2/2\sigma^2}$ . Here  $\mu$  is the mean, or average, of the distribution and  $\sigma^2$  is the variance, or mean square deviation.
- 17. For convenience, spin glasses are often labeled according to their coupling distributions; hence a spin glass in which the couplings are taken from a  $\pm J$  distribution is called a  $\pm J$  spin glass, and one in which the couplings are taken from a Gaussian distribution is called a Gaussian spin glass.
- 18. This remains a basic assumption in the field but is not accepted by all.
- 19. A coupling is *satisfied* when the spins at its endpoints are chosen so as to minimize their coupling energy. A ferromagnetic coupling is therefore satisfied if the spins at its endpoints are parallel, an antiferromagnetic coupling if they're antiparallel.
- 20. Frustration can be alternatively defined with respect to free energy fluctuations incurred when two blocks of spin glass are put together and the free energy is thereby minimized [75]. Here we confine

- ourselves to the simpler geometric interpretation [76] described in the text.
- 21. This is known as the *Mattis model* [77]. It is an easy exercise to show that (4.4) never occurs in such a model; try it.
- 22. For example, by studying a material whose interactions are strong within a line or plane and weak in other directions.
- 23. However, it doesn't display all of the experimental features of laboratory spin glasses, in particular, a specific heat that is nonsingular at  $T_f$ .
- 24. Clearly, an experimental test consisting of direct observation of spin time correlations would be difficult if not impossible to carry out, so, as usual, we rely on other observations, such as divergence of thermodynamic functions at the phase transition.
- 25. The time averaging implied in (4.5) is more usually represented in thermodynamic terms, but this requires the notion of a *pure state*, which we defer to section 7.2.
- 26. Spin-flip symmetry is an example of a *discrete* symmetry, since an Ising spin has only two possible states. This is to be distinguished from *continuous* symmetries, such as translational or rotational, discussed previously.
- 27. In an Ising model, where each spin can take on one of only two possible orientations, this space would be an *N*-dimensional hypercube, where each vertex of the hypercube describes one of the 2<sup>N</sup> possible configurations of all *N* spins.
- 28. In the probabilistic sense, that is, all except for a set of measure zero.
- 29. We will encounter the concepts of fixed point and basin of attraction again when we discuss neural networks in section 6.2.
- 30. To avoid complicating the discussion, we ignore "domain wall states"; see [82].
- 31. We emphasize that this is at best a picturesque description. Precise definitions of ground states are presented and discussed in chapter 7.

- 1. In fact, most statistical mechanical models have an *upper critical dimensionality*—usually 4 or 6 for spin systems, depending on the precise model—above which mean field theory becomes exact even at criticality. While fluctuations still exist, they are too weak compared to other factors to alter the nature of the critical point in higher dimensions. See, for example, [86, 87].
- 2. For example, a directly formulated mean field theory of spin glasses was constructed and analyzed by Thouless, Anderson, and Palmer [88].
- 3. If the couplings were all ferromagnetic, the normalization factor would be 1/N. Here, however, the couplings have random signs, so the N-1 interactions behave roughly like N-1 coin flips, giving an imbalance of  $O(\sqrt{N})$  (for N large) between positive and negative energy contributions.
- 4. This is needed to ensure that, just like energy, when you combine two smaller systems into a larger one, the resulting entropy is the sum of those of the component subsystems.
- 5. For those more mathematically inclined, a thermodynamic state can equivalently be thought of as a complete collection of all possible k-spin equal-time correlation functions for  $k = 1, 2, 3, \ldots$
- 6. We can now also refine our notion of phase transition: a sharp change from one thermodynamic state to another as temperature, pressure, or field is varied.
- 7. This interpretation of Parisi's solution of the SK model was worked out over a period of five years or so by many groups. Some (but far from all) of the fundamental papers include [93–97]; see also [98–100].
- 8. More generally,  $\langle \sigma_{i_1} \sigma_{i_2} \dots \sigma_{i_k} \rangle_{\alpha} = -\langle \sigma_{i_1} \sigma_{i_2} \dots \sigma_{i_k} \rangle_{\tilde{\alpha}}$  for k odd, and  $\langle \sigma_{i_1} \sigma_{i_2} \dots \sigma_{i_k} \rangle_{\alpha} = \langle \sigma_{i_1} \sigma_{i_2} \dots \sigma_{i_k} \rangle_{\tilde{\alpha}}$  for k even.
- 9. More precisely, a pure thermodynamic state.

- 10. This sort of behavior, intermediate between very simple and ordered, on the one hand, and completely random and/or chaotic on the other is characteristic of many complex systems.
- 11. The Dirac  $\delta$  function is a generalized function with the properties that  $\delta(x) = 0$  for  $x \neq 0$ ,  $\delta(0) = \infty$ , and  $\int_{-\infty}^{\infty} \delta(x) \, dx = 1$ . In other words, it's an infinitely high, infinitely narrow spike at the origin containing area one. Clear?
- 12. If you don't like or are confused by Dirac  $\delta$  functions, (5.4) simply means that the probability of the overlap taking on the value q is given by  $\sum_{\alpha\beta:q_{\alpha\beta}=q}W_{\alpha}W_{\beta}$ .
- 13. This situation can be generated using free or periodic boundary conditions, in a manner to be discussed in section 7.4.
- 14. Note that the first condition follows from the other three. To see this, set x = z.
- 15. Assuming that relations between relatives remain purely of the amicable kind.
- 16. Actually, it's the *distances*  $d_{\alpha\beta} = q_{EA} q_{\alpha\beta}$  that have the ultrametric structure, but for our purposes here, this is a detail.

- 1. An up-to-date and accessible introduction to many of the topics covered in this section, and much else besides, is provided by Moore and Mertens [114].
- 2. The precise mathematical formulation of this and related problems requires specification of a fixed *encoding scheme* that maps the input of an instance onto a finite string chosen from a finite alphabet, all in a clearly prespecified way. Here, however, we will avoid the mathematical niceties in order to keep the discussion informal.
- 3. One has to be a little careful, though. An algorithm whose time complexity is  $O(N^{100})$  is still formally polynomial time, but its usefulness for any realistically sized problem is no better than an exponential time algorithm. And even for more reasonable single-digit polynomial exponents, which characterize most polynomial time algorithms, an exponential time algorithm can still be faster for small to moderate N.

- 4. Details can be found in [115].
- 5. As of this writing.
- 6. If *NP*-complete problems are indeed intractable, it does *not* follow that  $P \cup NP$ -complete = NP; there would also exist exist problems that are neither *NP*-complete nor in P [117, 118].
- 7. More precisely, NP-hard, meaning at least as hard as NP-complete.
- 8. Interestingly, the problem of finding the ground state of a *two*-dimensional EA Ising spin glass belongs to *P*. But before you draw any conclusions, note that the same problem in two dimensions with *two* layers is *NP*-complete. The significance, if any, of all this remains unclear.
- 9. A picturesque way of seeing this, at least in a cartoon-sketchy sort of way, is suggested in figure 4.7. The analogy of a rapid cooling is to start at a random position well above the landscape and then to drop straight down. You may land in a low-lying valley if you're lucky, but you're more likely to end up in a higher-lying one.
- 10. Note that the zero-temperature dynamics described in section 4.9 is just the  $T \rightarrow 0$  limit of this procedure.
- 11. Something to contemplate the next time you pack the trunk of your car for an extended trip [123].
- 12. Remember, this was in the early 1980s!
- 13. As we saw in section 5.2, this rescaling of the coupling magnitude is necessary to obtain a cost per vertex that has a limiting value as  $N \to \infty$ .
- 14. For smaller values of *p* the agreement was less good, probably because of large sample-to-sample fluctuations.
- 15. For readers unfamiliar with the basic notions of neurons, such as firing, synapses, excitation, and inhibition, brief definitions are provided in the glossary.
- 16. Note that p=1 corresponds to the Mattis model (section 4.6). A model with p=2, which also has no frustration and is equivalent to a ferromagnet, had also been proposed and solved earlier by van Hemmen [144]. When p>2 things become much more complicated—and therefore interesting.

- 17. Given the nonbiological nature of the model at this point, we prefer to call the  $\sigma_i$ 's "elements" rather than "neurons."
- 18. The symmetry of the synaptic matrix  $J_{ij}$  ensures that the only attractors will be fixed points. If the symmetry assumption is dropped, it's possible to have limit cycles or other non-fixed-point attractors.
- 19. Or most *i*, in which case the fixed point will strongly correlate with the stored pattern but will have a few errors. See figure 6.5.
- 20. A trivial kind of spurious state would involve a global flip of all the  $\xi_i^{\mu}$ , but these are uninteresting.
- 21. For those familiar with the language of phase transitions, this is a *first-order* transition, as opposed to that noted earlier for fixed p at  $T_c = 1$ , which is second order.
- 22. As in biological neurons.
- 23. This is implemented by connecting a resistor with resistance  $R_{ij}$  between one of the outputs of amplifier j and the input of amplifier i; then  $|T_{ij}| = 1/R_{ij}$ . If the synapse is excitatory  $(T_{ij} > 0)$ , the resistor is connected to the normal output of amplifier j, and if it's inhibitory  $(T_{ij} < 0)$ , it's connected to the inverted output of j. See figure 6.8 for details.
- 24. This is related to a well-known biophysical model of neurons known as the Hodgkin-Huxley model [154].
- 25. This modifies the energy function by adding a "penalty term" if this condition is violated.
- 26. One of the founders of modern quantum mechanics.
- 27. At the time Schrödinger wrote this, it was still unclear whether the hereditary material consisted of proteins or nucleic acids, but the idea applied equally well to both.
- 28. The better-known hemoglobin molecule, found in red blood cells and which picks up, transports, and releases oxygen and carbon dioxide at the appropriate times, is essentially four myoglobin molecules loosely bound together.
- 29. A dalton is the same as an atomic mass unit, roughly the mass of a hydrogen atom.

- 30. The "compressibility," a measure of the (inverse) stiffness of the molecule, is between those of ice and lead [164].
- 31. Put another way, does myoglobin in its native state possess a rugged free energy landscape, as in figure 4.7?
- 32. One can now understand the exponential decay in time of N(t). Given that  $\exp(-\Delta F/k_BT) \ll 1$ , the escape becomes a Poisson process: many independent unsuccessful escape attempts must be made before a rare successful excursion occurs.
- 33. In solid state physics, this attenuation is quantified in the *Debye-Waller factor*; a derivation can be found in any solid state physics textbook. See, for example, [37].
- 34. In an insulator, the main contribution to the specific heat at low temperatures should scale as  $T^3$ , owing to lattice vibrations [37]. While this is also present in disordered systems, the linear contribution to the specific heat remained mysterious prior to the suggestion of TLS.
- 35. We use S rather than  $\sigma$  to emphasize that the physical quantity is not a spin but instead an atom or group of atoms that can be found in one of two states.
- 36. Again, the conclusions do not depend heavily on this assumption. Equations (6.16) and (6.17) result from a wide variety of distributions.
- 37. As noted, this is not a sharp temperature, but on laboratory timescales is reasonably well defined.
- 38. The genetic code of viruses can be based on either DNA or RNA. However, all viruses lack the cellular machinery for transcription—or anything else, for that matter.
- 39. By comparison, the current age of the universe is of order 10<sup>17</sup> seconds.
- 40. A more realistic estimate, based on the fact that most proteins take a few seconds to fold, and using a microsecond timescale for each attempt, would result in the protein's trying out roughly 10<sup>8</sup> configurations before finding the native state—enormously smaller than the total space of configurational possibilities.

- 41. Thermal denaturation is also a main factor behind the change in appearance of many food items on the application of heat in cooking.
- 42. Cold denaturation is also used in cooking, such as in the preparation of ceviche.
- 43. Discrete-state spin models where each spin can take on more than two possible states are known in the statistical mechanical literature as *Potts models*.
- 44. Indeed, it has justifiably been called "the simplest spin glass" by Gross and Mézard [193].
- 45. The connection between protein folding and glassy or spin glassy structure and dynamics was also pointed out by a variety of other groups; see in particular [192, 197, 198] and especially the review by Garel, Orland, and Thirumulai [199]. Spin glass ideas have also been applied to nonbiological polymers, especially with regard to cross-linking; see [200].
- 46. For excellent and relatively recent reviews, see [209, 210].
- 47. One well-known hypothesis is known as the "RNA world"; see, for example, [214–216].
- 48. Of course, most scientists working on the problem are interested in determining exactly this.
- 49. In so doing, the process generates a high Shannon, or information, entropy H [217]. In an N-bit string, this is defined to be  $H = -\sum_{i=1}^{N} p_i \log_2 p_i$ , where  $p_i$  is the probability of appearance of the ith bit. Shannon entropy becomes larger as the outcome becomes less predictable. This measure does not consider the significance or meaning of the outcome, only its unpredictability.
- 50. Surprise.
- 51. The assumption of a zero external field follows from the expected symmetry between  $ABAB\cdots$  and  $BABA\cdots$ .
- 52. The idea of modeling evolution as a sequence of point mutational steps that drives a system (in the case he was examining, a protein) uphill in fitness space is due to John Maynard Smith [227].
- 53. Kauffman refers to this as the *complexity catastrophe*.
- 54. Nongenetic inheritance of antibodies, as occurs in breast-feeding in mammals, can also take place.

- 1. Nevertheless, there has been theoretical work on this question. See [234–237].
- 2. Note that this notation can be used in any dimension d.
- 3. For the more mathematically inclined reader, we note that this assertion, and many others we'll be making later on, hold for all but a set of probability measure zero of coupling realizations. For brevity of presentation, this will be implicitly understood from now on.
- 4. We emphasize that avoiding the  $\pm J$  model is advisable only when dealing with ground state pair multiplicity; when dealing with other spin glass properties, such as the presence or absence of a phase transition, or dynamical properties at nonzero temperature, and so on, the  $\pm J$  model is perfectly fine.
- 5. For a more mathematical presentation of these concepts, see [238].
- 6. It should be clear that distinct ground state pairs must differ by the flip of an *infinite* set of spins.
- 7. This is possible because there are no loops in a one-dimensional lattice, hence no frustration in the infinite 1*D* spin glass. However, it would be incorrect to conclude that lack of frustration is sufficient to ensure that ground state behavior is trivial. Treelike structures known as *Bethe lattices* can be shown to have a complicated ground state structure.
- 8. Note that with free or periodic boundary conditions, finite-volume ground states still come in pairs. However, this will not be the case with a fixed boundary condition. We'll continue to refer to ground state pairs when talking in general, but want to point out this (not very essential) caveat.
- 9. In two dimensions, periodic boundary conditions are identical to wrapping the square into the geometry of a torus (doughnut).
- 10. Obviously, for a given window we can only consider  $\Lambda_L$ 's where L is large compared to the window size. Since  $L \to \infty$ , this never presents a problem for any fixed window, no matter how large.

- 11. Using compactness arguments, for you mathematicians out there. In a simpler setting such arguments show that for any sequence of real numbers  $x_1, x_2, \ldots$  whose values are always between -1 and +1, one can, by leaving some of them out, obtain a *subsequence*  $x_{n_1}, x_{n_2}, \ldots$  which converges to some number a (between -1 and 1, inclusive).
- 12. This interface has interesting geometric properties, which have been worked out in two dimensions; see [240] and [241].
- 13. This is a good thing, because it reflects the fact that strictly discontinuous behavior cannot occur in the physical world: a variable describing a classical physical system cannot jump from one value to another without passing through all those in between. Even so, although *technically* all thermodynamic functions vary smoothly through a change in phase in a macroscopic system, the variation is so rapid that for all practical purposes it can be treated as discontinuous.
- 14. This approach is usually described in terms of what are called the DLR (for Dobrushin, Lanford, and Ruelle [29]) equations.
- 15. Equivalently, a thermodynamic state can be defined by specifying the values of all 1-spin, 2-spin, 3-spin, ..., correlation functions, to be defined below.
- 16. A rather more physics-oriented example where mixtures occur is the  $d \geq 2$  homogeneous Ising ferromagnet at low temperature with periodic boundary conditions. Because of equal probabilities for spin configurations and their global flips, one gets a mixture, with W=0.5, of the positively and negatively magnetized phases (corresponding respectively to all +1 and all -1 boundary spins). A more subtle example occurs when d=2 and the boundary condition on  $\Lambda_L$  is +1 on the northern "hemisquare" and -1 on the southern. Here, one gets the same limit as for periodic boundary conditions, but for different reasons—see [245].
- 17. For a more complete and more precise discussion of pure and mixed thermodynamic states, and why the positive and negative definitions are equivalent, the mathematically inclined reader may look at [29].

- 18. One can also have an analogous integral of pure states in a continuum decomposition.
- 19. Of course, if  $\rho$  is itself pure, then the sum consists of a single term with weight one.
- 20. Here's a geometric analogy for pure and mixed states. A convex region of the plane is one where a line segment connecting any two points in the region stays entirely inside that region. Now consider three convex regions of the plane: (a) a finite straight line segment, (b) a finite triangular region, and (c) a circular disk. In this example, the analogs of the pure states are the boundary points, except those in the interior of a boundary line segment, and all other points in the convex region are mixed states. Then there are two pure state points in (a), three in (b), and a continuum (all points on the circumference) in (c). Now note that for (a) and (b) there is a *unique* decomposition for any point, as in (7.4), but not so for (c). The idea is that the family of thermodynamic states is geometrically like a single point in zero dimensions, a line segment in one, a triangle (but no other polygon) in two, and in higher dimensions is "pyramid-like."
- 21. And to more detailed versions, such as *which* types of pure and mixed states appear if one does not allow all possible boundary conditions but only "reasonable" ones like periodic.
- 22. In the SK model, where there is no geometry and therefore no boundary, this issue does not arise; one simply uses all the spins in the system.
- 23. This is not as exotic as the spin glass would be if it were to have many pure states. In the spin glass case, these many pure states would all be equivalent and equally likely to appear, whereas in the ferromagnet the uniformly magnetized, translation-invariant states are clearly special.
- 24. A shorthand way to say this is that the  $d \to \infty$  limit of the spin glass is *singular*.
- 25. As in the droplet/scaling scenario, if different choices of i and j give the *same* overlap value, then the corresponding probabilities  $W_i W_j$  should be added to give the overall probability for that overlap

- value. This feature will not be made explicit in our formulas but should be understood.
- 26. That is, quantities depending on only a finite number of spins.
- 27. To be more precise, it *would* be inherited if  $\rho_{\mathcal{J}}$  is constructed by an  $L \to \infty$  limit with periodic boundary conditions on  $\Lambda_L$  and *should* be valid more generally.
- 28. For you mathematical types, this is a consequence of the *translational ergodicity* of the disorder distribution. For nonmathematical readers this conclusion may seem mysterious. It rigorously follows from what is known as the *ergodic theorem*. What seems to be the earliest discussion of this theorem in the setting of averaging over translations is due to N. Wiener [254].
- 29. Recall that all statements of this type are true for all but a set of measure zero.
- 30. For those of you familiar with probability theory, you may wonder why a similar argument doesn't apply to the SK model. Here there is no translational symmetry, of course—there isn't even any geometry—but there is something similar: a permutation symmetry among the couplings. The point here is that zero-one laws of the type used to reach the "no non-self-averaging" conclusion for the EA model work only on functions of infinite numbers of random variables—in the spin glass case, therefore, for infinite systems only. Infinite-volume thermodynamic states make sense for the EA model and are explicitly constructible [253], but they make no sense for the SK model, as discussed in section 7.11. These considerations led to the revision, which we call the "nonstandard RSB model" (section 7.9), of the usual expressed view of RSB; so, if you prefer, you can think of the result described in this section as clarifying and limiting what RSB can and cannot mean when applied to the EA model.
- 31. In fact, with a little more work, it can be extended to other boundary conditions as well [241].
- 32. And it will, if droplet/scaling is correct.
- 33. More technically, from a metastate viewpoint we think of  $(\rho_{\mathcal{J}}^L$  and  $\mathcal{J})$  together as a random pair; this pair should have as  $L \to \infty$  a

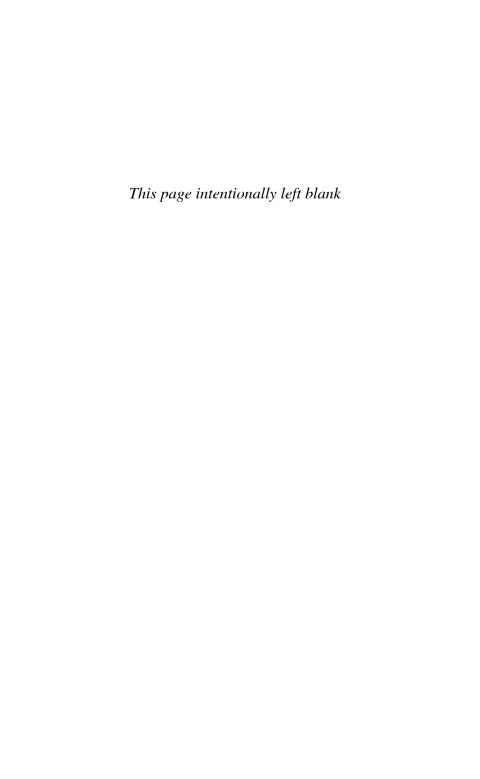
- limit (known as a *distributional* limit) ( $\tilde{\rho}_{\mathcal{J}}$ ,  $\mathcal{J}$ ), in which  $\tilde{\rho}_{\mathcal{J}}$  is not a single thermodynamic state like  $\rho_{\mathcal{J}}$  depending on  $\mathcal{J}$  but rather a *random* thermodynamic state whose distribution is a metastate  $\kappa_{\mathcal{J}}$  depending on  $\mathcal{J}$ .
- 34. This is because flipping boundary conditions on a large  $\Lambda_L$  should change the  $\alpha_i$ 's and  $W_i$ 's in the (approximating) pure state decomposition for that L to very different  $\alpha_i$ 's and  $W_i$ 's. For more detailed arguments, see [238, 239, 266].
- 35. Recall from the preface that TNT stands for *tr*ivial edge overlap, *nontr*ivial spin overlap.
- 36. This is for essentially the same reason as that given in section 7.1 for there only being a single pair of ground states in one dimension. Now, though, instead of a "weak link" wandering off to infinity as one increases system size, the lower-dimensional *interface* wanders off to infinity.
- 37. This can lead to some very strange effects, as shown in [274].
- 38. It's really the statistical independence of the *signs* of the couplings that's crucial. A disordered infinite-range ferromagnet with all couplings positive but with random magnitudes would behave pretty much like a homogeneous ferromagnet.
- 39. A concise tabular summary of the fundamental differences among these four pictures can be found in [276].
- 40. But if you're interested in speculations based on very little, but that at least are fun, take a look at [44,284].

- 1. See also the suggested books on complexity cited in the introduction.
- 2. Our choice of three out of many potential candidates is undoubtedly idiosyncratic and subject to valid dispute. We'd love to hear your views when we have some free time.
- 3. Indeed, one can argue that the skill of teasing out a few relevant variables from the tangled mass of complicated features of a system,

rather than technical mathematical ability, is what sets the most successful physical scientists apart from their peers.

- 4. And vague.
- 5. The matrix displayed here is not quite the same as that constructed in the Parisi RSB scheme, which differs in several respects (e.g., in having zeroes along the diagonal). But the spirit is the same.
- 6. Transition matrices describing an "ultrametric dynamics" have a similar structure; see [182–184].
- 7. We've arranged the hierarchical ordering of science slightly differently from Anderson's, but not in a serious way.
- 8. This viewpoint is probably not as widely held—at least not openly—as it was at the time Anderson wrote his article. Still, use of terms like "Theory of Everything" to describe a theoretical unification of all forces and matter is perhaps a modern example of this attitude. While catchy, such names are misleading, however important and (let's say it) fundamental a unification theory would be.
- 9. As many have noted before us, this is one case where using just the acronym for broken symmetry leads to unfortunate consequences. Or appropriate ones, depending on your point of view.
- 10. Reservations were expressed in the paper as to the depth of the broken symmetry "analogy" in particle physics. Forty years later, it's probably safe to say that those reservations can be dropped.
- 11. Recall the discussion in the introduction regarding the "edge of chaos" and related concepts.
- 12. To get an idea of the wide range of viewpoints on the subject, see the special *Science* issue on complexity (April 2, 1999).
- 13. Interestingly, Shannon's paper appeared at roughly the same time as Weaver's.
- 14. Crutchfield and Shalizi [298] have criticized the notion of thermodynamic depth by pointing out difficulties in precisely defining "historical paths." It's probably fair to say, though, that all proposed measures of complexity suffer from precise definitional problems in one way or another.
- 15. In fact, some, such as algorithmic complexity, are known to be Turing-uncomputable for most specific strings.

- 16. Parts of this section are adapted from [275].
- 17. Moreover, the combined presence of disorder and frustration must be at least partly—if not wholly—responsible for the presence of a large number of interdependent collective coordinates, possibly on multiple length- and timescales, that determine spin glass equilibrium and nonequilibrium behavior. This property would likely give rise to a large Grassberger-Crutchfield-Young statistical complexity (as discussed in the previous section) for spin glasses. We thank an anonymous referee for pointing this out.
- 18. Or, more precisely, distance between states as measured by overlaps.
- 19. The reason why mean field theory could—or even should—fail to describe short-range spin glasses in any finite dimension was discussed in section 7.11.
- 20. And, as we've emphasized in section 7.10, this by itself is *not* equivalent to replica symmetry breaking holding for these systems; RSB describes a way in which many pure states are *organized*. If many pure states do occur, their most likely manner of organization is through the very different chaotic pairs scenario.
- 21. At a very deep level. Even if true, this doesn't preclude useful analogies and transference of methods to solve carefully circumscribed problems, as we've seen throughout this book.



### GLOSSARY

Few readers will be conversant with all of the subjects treated in this book, so we've provided a glossary of some of the technical terms. The definitions below are informal and very brief; more detailed expositions can be found in the text. The section in which a term is discussed in detail (or in which references doing so can be found) appears in parentheses following the definition.

- **Aging** A nonequilibrium dynamical phenomenon wherein a system "remembers" how long it was held at a fixed temperature or field (section 4.3).
- Amino acids The building blocks of proteins, each consisting of an amine group, a carboxylic acid group, and a side chain that distinguishes one kind of amino acid from another (section 6.3.1).
- **Antibody** A protein "evolved" by the immune system to bind to antigens and thereby incapacitate foreign invaders such as bacteria or viruses (section 6.4.3).
- Antiferromagnetism A type of magnetic ordering wherein the ground state aligns neighboring spins antiparallel to each other (if geometry allows) (section 3.6).
- Antigen A molecule that triggers the immune response (section 6.4.3).
- Associative (or content-addressable) memory A memory addressed by content rather than by a fixed address, that is, where clues

266 Glossary

or associations are vital in referencing, and thereby retrieving, the memory. The term is used both in neural network theory and in computer science (section 6.2.2).

- Basin of attraction (in thermodynamics) (1) Of a ground state: at zero temperature, the set of configurations that flow to a fixed point under almost every realization of the zero-temperature dynamics. (2) Of a pure state: the set of configurations that evolve toward a pure state under almost every realization of the positive-temperature dynamics (section 4.9).
- **Bloch wave** In quantum mechanics, the wavefunction of a particle in a periodic potential. The wavefunction is characterized by a function with the periodicity of the potential multiplied by a plane wave, and therefore extends over the entire lattice. Bloch waves are of primary importance in solid state physics, where they describe the wavefunction of an electron in a crystal (section 2.3).
- **Boltzmann distribution, factor** For a system in equilibrium at temperature T, a specific configuration with energy E appears with probability  $P(E) = \frac{1}{Z}e^{-E/k_BT}$ , where  $Z = \sum_{\text{all configurations}} e^{-E\{\text{configurations}\}/k_BT}$ . The term  $e^{-E/k_BT}$  is called the *Boltzmann factor*, and a probability distribution in which configurations are distributed by the above law is called a *Boltzmann distribution* (section 1.5).
- Broken spin-flip symmetry A situation in which an Ising spin system has (1) a Hamiltonian  $\mathcal{H}$ , in which a change of sign of every spin leaves the energy unchanged, and (2) two or more low-temperature phases, each having the property that the time-averaged values of individual spins (or products of odd numbers of spins) are nonzero (section 4.8).
- **Broken symmetry** In condensed matter physics, a situation in which the ground state or low-temperature phase of a system displays less symmetry than the Hamiltonian (section 1.3).
- **Boundary condition** A specification, inserted by hand, of the spin configuration on the boundary of a finite volume (section 7.1).

- **Calmodulin** A protein that binds calcium (section 6.3.1).
- Capacity (of neural network) The maximum number of memories that can be stored in a neural net without significant retrieval error (section 6.2.2).
- Chaotic pairs One possible scenario for the low-temperature phase of short-range spin glasses in which each observed thermodynamic state consists of a single pair of spin-reversed pure states, but there are many distinct pure state pairs (section 7.10).
- Chaotic size dependence (CSD) The absence of an infinite-volume limit for a sequence of finite-volume thermodynamic states. The presence of CSD signals the presence of multiple thermodynamic states (section 7.8).
- Combinatorial optimization problems A class of graph-theoretic problems in computer science in which the number of possible solutions grows extremely rapidly with the size of the input, so that an exhaustive search of all possible solutions is not a viable means of finding an optimal solution (section 6.1.1).
- Condensed matter physics The physics of how matter organizes itself on a macroscopic scale; more specifically, the physics of solids, liquids, superfluids and superconductors, liquid crystals, magnetic materials, and other states of matter where interactions between the microscopic constituents play a primary role in determining the macroscopic properties (chapter 1, introduction).
- **Configuration** A complete specification of the microscopic state (position and momentum for atoms, orientation for spins) of each of the many degrees of freedom in a system (section 1.2).
- Conformational substates Locally stable protein configurations, all with the same tertiary structure but differing in the time-averaged spatial location of a non-negligible fraction of the protein's atoms (section 6.3.1).
- **Conserved quantity** A physical quantity that remains fixed for all time (section 1.1).
- Content-addressable memory See Associative memory.

268 Glossary

- Correlation function (in spin glasses) The expectation (i.e., average value) in a given thermodynamic state of the product of a finite set of spins (section 7.2).
- Coupling realization A complete specification of every coupling value (sign and magnitude) in a particular spin glass sample. In theoretical spin glass models, the coupling values are selected according to a prespecified probability distribution (section 4.5).
- **Crystal** A solid in which the atoms or molecules are arranged in a periodic (i.e., endlessly repeating) lattice structure (section 1.2).
- de Almeida–Thouless (AT) line The boundary between the spin glass phase and the paramagnetic phase in the h–T plane (section 5.3).
- **Debye-Waller factor** A quantity describing the degree of attenuation of X-ray scattering from a crystal caused by thermal or other motion of the atoms (section 6.3.1).
- **Deep quench** Rapid cooling of a material from a very high temperature to a very low one (contrast with Quasi-static process, q.v.) (section 4.3).
- **Degrees of freedom** Informally, the microscopic constituents of a macroscopic system, for example, atoms in a solid, liquid, or gas, or spins in a magnet; more precisely, the *coordinate variables* specifying the state of these constituents at any moment. For example, in a glass of water, each  $H_2O$  molecule, treated as a point particle, has three position coordinates, x, y, and z, and three momentum coordinates,  $p_x$ ,  $p_y$ , and  $p_z$ . For a liquid with N molecules, there are therefore 6N degrees of freedom (section 1.2).
- **Denaturation** A process that destroys the tertiary structure of a protein. *Thermal* denaturation destroys the tertiary structure through heating, *cold* denaturation does so through chemical means (section 6.3.2).
- **Disorder chaos** Reflects sensitivity of the ground state(s) or pure state(s) to coupling realization. *Disorder chaos* occurs when an arbitrarily small change in the couplings leads to large-scale changes in the thermodynamic state(s) at fixed temperature (cf. Temperature chaos) (section 7.12).

Glossary 269

- **Dispersal of the metastate** A situation wherein the metastate is supported on more than one thermodynamic state, with different thermodynamic states appearing in different subsets of volumes as a consequence, leading to *chaotic size dependence* (q.v.) (section 7.9).
- **Droplet/scaling scenario** A scenario for short-range spin glasses in finite dimensions in which the low-temperature phase is characterized by a single pair of spin-reversed pure states, with large-scale excitations above a ground state governed by droplets of reversed spins whose energy scales as a power law in their linear size (section 7.4).
- Edwards-Anderson (EA) model A simplified theoretical model of short-range spin glasses in finite dimensions, specified by the Hamiltonian (4.2), where each spin is coupled only to its nearest neighbors and the couplings are (usually independent, identically distributed) random variables determined by a given probability distribution (section 4.5).
- Edwards-Anderson order parameter An order parameter given by (4.5). If nonzero, it implies spin freezing and broken spin-flip symmetry (in an Ising model) or broken rotational symmetry (in a continuous spin model) (section 4.8).
- Emergence The appearance of new collective phenomena, not apparent or predictable from a detailed knowledge of a system's microscopic constituents, arising from an interacting collection of a large number of these constituents (introduction and section 8.3.2).
- **Energy landscape** Roughly speaking, a very high-dimensional "graph" of the energy of a system as a function of the system's configuration (section 4.9).
- **Entropy** A measure of the disorder of a system. More precisely, a dimensionless number proportional to the logarithm of the number of microscopic configurations all having the same energy (within an infinitesimally narrow range) (sections 1.5 and 5.3).
- **Equilibrium** In thermodynamics, a situation wherein the macroscopic properties of a system are unchanging in time (for a suitably defined period) and can be described by a handful of variables (e.g., internal energy, volume, magnetization) that depend only on the internal

state of the system and not on its history, manner of preparation, and so forth (section 2.1). In statistical mechanics, a system at fixed temperature whose energies are distributed according to the Boltzmann distribution (section 1.5).

**Ergodic theorems** A class of theorems asserting (roughly speaking) that for random variables chosen from certain probability distributions, the time average or space average of functions on these random variables equals the average of these same functions over the probability distribution (section 7.7).

Excitation In condensed matter physics, usually refers to a configuration with energy slightly above the ground state (section 1.4). In neural science, an increase in the firing rate of a neuron (cf. Inhibition), usually caused by a stimulus from another neuron across a synapse (section 6.2.1).

Exponential-time algorithm See Time complexity.

**Ferromagnetism** A type of magnetic ordering in which the ground state has all spins aligned (section 3.5).

Firing (of a neuron) Following activation above a certain threshold, the sending of an electrical or chemical signal by a neuron to others connected to it (section 6.2.1).

**Fixed boundary condition** A type of boundary condition that assigns each boundary spin a prespecified value, which thereafter remains fixed (section 7.1).

**Fixed point** In dynamical systems, a point that remains invariant under noise-free dynamics (section 4.9).

Folding funnel A proposed form of the free energy landscape for protein folding in which the native state lies at a free energy minimum and the landscape, though rugged, tends to guide the protein toward its native state as folding proceeds (section 6.3.2).

Free boundary condition The boundary condition in which every boundary spin is free to take on any of its allowed values (section 7.1).

Free energy A thermodynamic variable equal to E-TS, where E is the system's internal energy, T its temperature, and S its entropy. (Note: This is a particular kind of free energy, called the *Helmholtz* free energy. There are other kinds also, but those won't be considered

- here.) In thermodynamics, the free energy is the energy available for a system to do useful work. In statistical mechanics, it is the quantity that is minimum for a system in thermal equilibrium at fixed temperature (section 1.5).
- **Frustration** A situation wherein not all of the constraints on a system can be simultaneously satisfied. In a spin glass, frustration refers to the fact that the ground state cannot satisfy all of the couplings (section 4.6).
- Gaussian distribution A probability distribution in which the continuous random variable X is distributed according to  $P(x) = \frac{1}{\sqrt{2\pi\sigma^2}}e^{-(x-\mu)^2/2\sigma^2}$ . Here  $\mu$  is the mean, or average, of the distribution and  $\sigma^2$  is the variance, or mean square deviation. Also known as the normal distribution or bell curve (section 4.5).
- Gibbs measure, state See Thermodynamic state.
- **Glass** A solid (on human timescales) in which the atoms or molecules are "stuck" in random locations, with no long-range order; a noncrystalline solid (section 2.2).
- **Glass transition** The (nonthermodynamic) transition from a viscous liquid to a glassy state where macroscopic flow ceases on experimental timescales (section 2.2).
- Goldstone modes Low-energy, long-wavelength excitations above a broken-symmetric ground state. An example is sound waves in a crystal (section 1.4).
- **Graph** A set in which either some or all elements (called *nodes* or *vertices*) are connected pairwise through *links* (or *edges*) (section 6.1.5).
- **Graph partitioning** A set of graph theory problems in which a given graph with V vertices and E edges must be partitioned in a specified manner. The simplest version is where the vertices (whose total number is even) are to be divided into two equal sets, with the goal being to minimize the number of edges passing between the two sets (this is known to be an NP-complete problem) (section 6.1.5).
- Ground state In finite systems, the configuration(s) with lowest energy (consistent with the given boundary conditions). In infinite spin systems, the configuration(s) whose energy cannot be lowered by changing any finite set of spins (section 7.1).

- **Hamiltonian** A function on configurations that assigns an energy to each configuration (section 1.2).
- **Hebb rule** A model for plasticity (i.e., change) in neural networks in which repeated firing across synapses strengthens the connection between the associated neurons (section 6.2.1).
- **Hopfield model** An artificial neural network model for studying associative memory, in which neurons are treated as binary elements with symmetric connections and a Hebbian learning rule. Memories are provided as inputs through a connectivity matrix between neurons (section 6.2.2).
- **Information entropy** *See* Shannon entropy.
- **Inhibition** In neural science, a decrease in the firing rate of a neuron (cf. Excitation), usually caused by a stimulus from another neuron across a synapse (section 6.2.1).
- **Interface** (between ground states) The set of couplings that are satisfied in one ground state and not the other (section 7.1).
- **Intractable** (in computer science) Denotes a problem for which no polynomial time algorithm can be found (section 6.1.2).
- Ising model A statistical mechanical model in which the degrees of freedom are binary variables. It was originally proposed as a simplified model for ferromagnetism, in which the spins were taken to be discrete variables having two states, up or down, or mathematically ±1. The Ising model is widely used in statistical mechanics, not only for magnetic systems such as ferromagnets, anti-ferromagnets, and spin glasses but also for problems in nonmagnetic systems, such as lattice gases, binary alloys, and many others (section 4.5).
- **Isotropic** In application to physical law, denotes a law that is invariant with respect to changes in direction; in application to physical systems, denotes a system that is uniform in all directions (section 1.1).
- **Kondo effect** A minimum in the resistivity of dilute magnetic alloys at low temperature (section 4.1).
- **Lattice constant** The shortest distance in a given direction in which a lattice repeats itself (section 1.1).
- Levinthal paradox The seeming paradox that, given the enormous number of possible spatial configurations of a primary sequence

of amino acids, a protein could not possibly find its native state on any reasonable timescale by randomly searching among possible configurations. This is really not a paradox but rather a convincing estimate (section 6.3.2).

- Lin-Kernighan algorithm One of the most efficient algorithms currently known for attempting to solve the Traveling Salesman Problem (section 6.2.3). (Note: there also exists a Kernighan-Lin algorithm for solving graph partitioning.)
- **Localization** The nonperiodic behavior of an electron wavefunction in a disordered solid; in particular, the wavefunction magnitude (and therefore the probability of finding the electron) is maximum in a local region of the solid and falls off away from it (section 2.3). (Note: This is *Anderson localization*. There are other kinds of localization, which are not dealt with here.)
- **Long-range order** In condensed matter systems, the phenomenon in which information about the organization of the degrees of freedom in one region provides information about the organization in the same system arbitrarily far away. When long-range order is *not* present, such information decays rapidly (usually exponentially) with distance (section 1.2).
- Magnetic susceptibility See Susceptibility.
- **Magnetization** A thermodynamic variable that provides the spatial average of the orientation of the time-averaged spin degrees of freedom in a magnetic system (section 3.4).
- Maturation (of immune response) The increase in time, usually over a matter of days, of affinity (i.e., binding constant) of antibodies to antigens, through a kind of somatic-cell selection (section 6.4.3).
- **McCulloch-Pitts neuron** An artificial neuron modeled as a binary logical unit, that is, having only two states, on or off (section 6.2.1).
- Mean field theory A simplified statistical mechanical modeling technique in which a system is treated as if the local environment at every point were the same. This must be done in a self-consistent way because, for example, in a magnetic system, the spins give rise to an average, or mean, internal field, which then acts back on the spins (section 5.1).

- **Metastate** A probability distribution over the thermodynamic states in a system (section 7.8).
- Metric space A set in which a distance function between the elements is defined. The distance function must satisfy certain properties: nonnegativity, zero distance only between a point and itself, symmetry, and triangle inequality (section 5.6.3).
- Metropolis algorithm A class of algorithms that constructs a Markov chain (a memoryless random process in which the state at step n + 1 depends only on the state at step n, and the transition rule and nothing else) designed to lead to an equilibrium (Boltzmann) distribution (section 6.1.4).
- **Mixed thermodynamic state** A thermodynamic state that can be uniquely decomposed as a convex combination of two or more distinct pure states (section 7.2).
- **Molten globule** A partially folded protein state containing most of the secondary structure but only part of the tertiary structure; an intermediate state neither native nor denatured (section 6.3.2).
- **Mössbauer effect** The recoilless emission and absorption of gammaray photons by the nuclei of certain atoms (particularly iron) bound in a solid (section 6.3.1).
- **Myoglobin** A compact, globular protein consisting of 153 amino acids, used to bind oxygen in muscle cells. A hemoglobin molecule is essentially four myoglobin molecules loosely bound together (section 6.3.1).
- Native state The biologically useful, fully folded tertiary structure of a protein; the three-dimensional structure a protein assumes when functioning properly within an organism (section 6.3.1).
- **Nearly decomposable system** Proposed by Herb Simon as a mathematical basis for the architecture of complex systems. A *nearly decomposable system* is built up through a hierarchical structure, with many subsystems that interact weakly with one another but whose components are strongly interacting within the subsystem itself. Each of the subsystems contains its own subsystems, through several levels (section 8.1.2).

- Neural computation (artificial) A (usually analog) computation using circuits designed to simulate highly interconnected neuronlike elements to solve problems in areas such as combinatorial optimization, pattern recognition, and others. Rather than using the standard algorithmic approach, the dynamics is intended to flow toward a fixed point representing an optimal or near-optimal solution (section 6.2.3).
- Neural network (or neural net) Either a biological network of neurons, connected through synapses, or, more commonly today, an artificial one consisting of elements ("neurons") connected in a prespecified way ("synapses") (section 6.2.1).
- **Neuron** A cell that forms the basic constituent of the nervous system of many animal species. Neurons are electrically excitable cells, using both electrical and chemical means to transmit signals (section 6.2.1).
- $NK \bmod e$  A spin-glass-like model due to Stuart Kauffman in which N denotes the number of degrees of freedom in the system and the tunable parameter K denotes the extent of interactivity of the system (section 6.4.2).
- Noise-free dynamics (also zero-noise or zero-temperature dynamics) Dynamical rules governing the evolution of a system in which each updating step that changes the energy occurs with either probability zero or one (section 4.9). (Note: This does not imply a complete absence of randomness: for example, in asynchronous dynamics in which each degree of freedom is chosen one at a time for possible updating, the order in which the degrees of freedom are chosen could be random.)
- **Non-self-averaging** The property of global thermodynamic quantities (such as the overlap function) depending on coupling realization, even in the thermodynamic limit (section 5.6.2).
- **NP** "Nondeterministic polynomial time," designating a class of combinatorial optimization problems. Roughly speaking, a problem belongs to *NP* if a guessed solution can be computationally verified (or discarded as incorrect) in polynomial time (section 6.1.2).
- **NP-complete** The subset (maybe—see  $P \neq NP$ ) of problems within NP having the property that every problem in NP can be polynomially

- reduced to them; roughly speaking, the "hardest" problems in the class NP (section 6.1.2).
- **Order parameter** A thermodynamic variable characterizing the manner of ordering in a system. The *amplitude* of an order parameter describes the *extent* to which symmetry is broken; its *phase* describes the exact *manner* in which it's broken (section 1.4).
- Overlap density A function specifying the probability that, if two spin configurations are chosen randomly from a mixed thermodynamic state, their spin overlap function takes on a given value (section 5.6.2).
- Overlap function See Spin overlap function.
- **P** "Polynomial time," designating a class of combinatorial optimization problems that can be solved using polynomial time algorithms (section 6.1.2).
- $P \neq NP$  The conjecture, widely believed to be true, that the set of problems in P is a proper subset of all those in NP. If true, this would mean that NP-complete problems are intractable (section 6.1.2).
- **Paramagnetism** The high-temperature phase of all magnetic systems, characterized by a zero value for the expectation (or average value) of every spin (section 3.3).
- Parisi order parameter Roughly speaking, the function describing the probability (when computed over *all* coupling realizations) that two randomly chosen spin configurations have a spin overlap equal to (or in some versions, less than or equal to) any specified value (more precisely, within an infinitesimal range of that value) (section 5.6.2).
- **Parisi solution** The statistical mechanical solution for the free energy of the low-temperature phase of the Sherrington-Kirkpatrick Ising model, based on a unique kind of symmetry breaking called *replica summetry breaking*. It is characterized by an infinite set of statistically equivalent pure states, a non-self-averaging of overlaps between these pure states, and an ultrametric structure in the space of pure states (section 5.6.2 and subsequent sections).
- **Periodic boundary condition** The boundary condition that requires each spin to take on the same value as that on the opposite boundary

- (but otherwise leaves the pair free to choose any of their allowed values) (section 7.1).
- Phase (of matter) A distinct form of organization of matter, represented in statistical mechanics by a pure thermodynamic state. Examples include crystals, liquids, gases, ferromagnets, paramagnets, and superconductors (section 1.5). (Note: Some people use "state of matter" for this, with "phase of matter" having a somewhat different meaning. But we use the two terms interchangeably.)
- Phase transition A sharp (in the thermodynamic limit) transition between two distinct phases of matter, characterized by discontinuous or singular behavior of certain thermodynamic functions (section 1.6).
- Plus or minus J ( $\pm J$ ) spin glass A spin glass whose couplings are chosen independently from an extreme bimodal distribution: +J with probability p and -J with probability 1-p. The most common case uses p=1/2, but the thermodynamic behavior as p varies has also been studied (section 4.5).
- Polynomial time algorithm See Time complexity.
- **Polynomial time reducibility** Problem *A* is *polynomial time reducible* to problem *B* if an algorithm solving every instance of *B* can be converted through a second, polynomial time algorithm to one that solves every instance of *A* (section 6.1.2).
- **Primary structure** The linear sequence of amino acids constituting a protein (section 6.3.1).
- **Principle of minimal frustration** The notion that evolution has engineered proteins so that their secondary structures favor their native structure; consequently frustration, though unavoidable to some extent, is minimized (section 6.3.2).
- **Proteins** Large biomolecules that are polymeric chains of amino acids, performing numerous functions in organisms: as catalysts for biochemical reactions (the *enzymes*); as intra- or intercellular structural supports; as transporters of ions, atoms, or molecules; as channels through which ions, atoms, or molecules can be transported; as signal carriers, and many others (section 6.3.1).

- **Protein folding problem** The problem of how a protein finds its tertiary structure given its primary structure (section 6.3.2).
- Pure thermodynamic state A thermodynamic state that *cannot* be written as a convex combination of distinct thermodynamic states. Equivalently, a thermodynamic state having the property that correlations between two regions (such as the covariance between the spin variables at two separated locations) increasingly decouple as the distance between them increases (section 7.2).
- Quasi-static process A process wherein temperature (or pressure, or field) is changed sufficiently slowly that the system essentially remains in thermodynamic equilibrium throughout the process (contrast with Deep quench, q.v.) (section 2.2).
- Quenched disorder Frozen-in disorder, usually but not necessarily following a deep quench (contrast with Thermal disorder, q.v.) (section 2.2).
- Random energy model A simple statistical mechanical model, due to Bernard Derrida, in which there are  $2^N$  states whose energies are taken to be independent, identically distributed random variables chosen from a Gaussian distribution. Called the "simplest spin glass" by Gross and Mézard (section 6.3.2).
- **Relaxational timescale** The characteristic time for a system to equilibrate after a perturbation, or otherwise relax back to its initial state (section 2.2).
- Remanent magnetization The magnetization that remains after an external magnetic field has been removed. Two kinds are important in spin glasses: *thermoremanent* magnetization (TRM), wherein a spin glass is cooled in an external field, after which the field is removed, and *isothermal remanent* magnetization (IRM), in which a spin glass is cooled in zero field, after which a field is turned on for a time and then removed, all at fixed temperature. The residual magnetization of the sample after the field has been turned off is the IRM (section 4.3).
- **Replica method** A procedure for computing the free energy in a system with quenched disorder. It involves computing a thermodynamic average over many independent copies, or *replicas*, of a system, and then taking the number of replicas to zero (section 5.4).

- Replica symmetry breaking (RSB) A novel kind of symmetry breaking in which a system distinguishes between initially identical replicas, presumably indicating the presence of many pure states (section 5.4).
- Ruderman-Kittel-Kasuya-Yosida (RKKY) interaction A long-range, oscillatory interaction between magnetic impurity spins localized in a nonmagnetic metallic host (section 4.4).
- Rugged landscape An energy landscape of a system possessing many metastable and/or stable states. Such a landscape is picturesquely thought of as having many "hills" (barriers) and "valleys" (stable or metastable states) (section 4.9).
- Satisfiability (abbr. SAT) A combinatorial optimization problem in which the variables are binary (1 or 0, corresponding to TRUE or FALSE), and an instance is a collection of *clauses* using the operations AND, OR, and NOT. An instance is *satisfiable* if there exists an assignment of values to all the variables such that all statements are TRUE. For example, (*a* AND *b*) AND (NOT *c*) is true if we assign the values TRUE to *a* and *b* and FALSE to *c*. *k*-Satisfiability is a special case in which all clauses contain *k* variables. Satisfiability was the first known example of an *NP*-complete problem (section 6.1.2).
- **Secondary structure** Localized spatial domains along partial segments of a protein; can be single helices, pleated structures, or other configurations (section 6.3.1).
- **Self-averaging** A thermodynamic quantity, such as energy per spin or free energy per spin, that is independent of coupling realization in the thermodynamic limit (section 5.6.2).
- Shannon entropy A measure of uncertainty or unpredictability of a string of bits (0s and 1s), given by  $H = -\sum_{i=1}^{N} p_i \log_2 p_i$ , where  $p_i$  is the probability of appearance of the *i*th bit. The higher the Shannon entropy, the greater the information content of a given string (section 6.4.1).
- Sherrington-Kirkpatrick (SK) model The infinite-range version of the Edwards-Anderson model, with the Hamiltonian given by (5.1) (section 5.2).

- Simulated annealing An algorithmic approach that treats combinatorial optimization problems as statistical mechanical problems, wherein a Metropolis algorithm is used to "cool" the system from high to low temperature. Here "temperature" is simply a parameter used to assign relative probabilities to configurations with different cost functions (section 6.1.4).
- **Space translation** Imagining every degree of freedom in a system moved simultaneously in space in exactly the same direction and by exactly the same amount (section 1.1).
- Specific heat (also known as heat capacity) The amount of heat needed to be added to a system to raise its temperature by a fixed amount (section 1.6).
- Spin The quantum mechanical degree of freedom that describes the intrinsic (i.e., independent of particle motion) angular momentum of an elementary or composite particle. Also used informally to denote the intrinsic magnetic moment associated with spin (section 3.1).
- **Spin overlap function** The product of the expectation values in two pure states of a single spin, averaged over all spins; provides a measure of similarity between the two pure states (section 5.6.1).
- **Spurious states** In Hopfield neural nets, unwanted fixed points that do not correspond to stored memories (section 6.2.2).
- **Statistical mechanics** The application of probabilistic methods to a large collection of degrees of freedom, with the aim of extracting the system thermodynamics (section 1.5).
- **Stochastic stability** A system exhibits *stochastic stability* when a certain set of perturbations to its Hamiltonian produces changes in its thermodynamic state(s) that vanish in the thermodynamic limit (section 7.12).
- **Susceptibility** The magnetic response of a system to an external magnetic field; more precisely, the change in its magnetization upon application of an infinitesimal external field (section 3.5).
- Symmetry (of a physical law) Invariance of a physical law following a coordinate transformation (i.e., a change in coordinate system) (section 1.1). (Note: This definition covers only what are known as *global* symmetries, in which the coordinates of every degree of

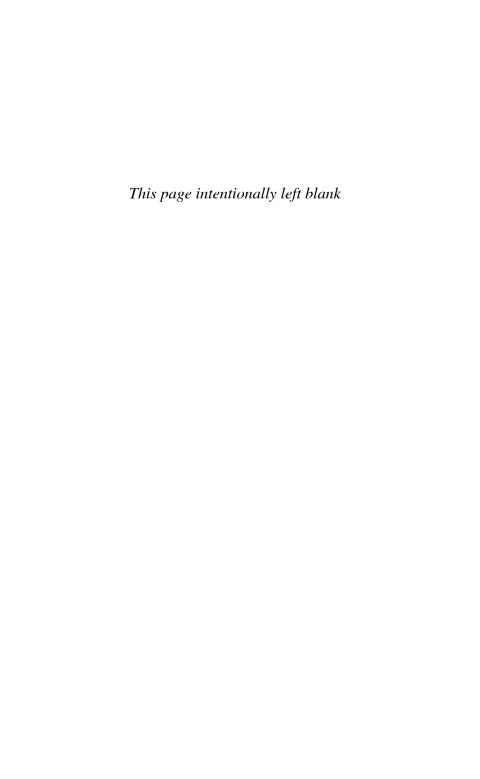
- freedom change by the same amount. There may also be local, or *gauge*, symmetries in which each particle or degree of freedom undergoes its own internal transformation; these are not discussed in the text.)
- Synapse A small gap between two neurons, through which signals are passed (using chemical or electrical means) from one neuron to another (section 6.2.1).
- **Temperature chaos** Sensitivity of the ground state(s) and/or pure state(s) to temperature. *Temperature chaos* occurs when an arbitrarily small change in the temperature leads to large-scale changes in the thermodynamic state(s) at fixed coupling realization (cf. Disorder chaos) (section 7.12).
- **Tertiary structure** The three-dimensional structure of a fully folded protein (section 6.3.1).
- Thermal disorder Disorder induced by high temperature, in which degrees of freedom are rapidly flitting in and out of different configurations (cf. Quenched disorder) (section (5.1)).
- Thermodynamic hypothesis (in protein folding) The conjecture that the native state of a protein is a minimum of the thermodynamic free energy (section 6.3.2).
- Thermodynamic limit The limit  $N \to \infty$ , where N is the number of degrees of freedom of a system (section 7.6).
- Thermodynamic state In a spin system, a probability distribution over all spin configurations; or equivalently, a list of all 1-spin, 2-spin, 3-spin, etc., correlation functions. Also called Gibbs state or Gibbs measure (sections 5.5 and 7.2).
- Time complexity (of an algorithm) The amount of time an algorithm takes to run as a function of the problem's input size. Two important cases are *polynomial time* algorithms, whose running time grows no faster than the input size raised to a power, and *exponential time* algorithms, whose running times grow exponentially with input size (section 6.1.2).
- Time reversal A coordinate transformation in which the time variable t is switched to -t wherever it explicitly appears in a physical law or equation of motion (section 1.1).

- Time translation A coordinate transformation in which the time variable is shifted by a constant amount, that is,  $t \to t + c$ , where c is a (positive or negative) constant, wherever it explicitly appears in a physical law or equation of motion (section 1.1).
- TNT scenario A scenario for the low-temperature phase of short-range spin glasses in finite dimensions in which large-scale excitations (i.e., excitations involving flipping a number of spins that grows with the system size) above the ground state have energies that remain of order one regardless of the excitation's characteristic size, and the boundary of the excitation is of lower dimensionality than the dimensionality of the system (section 7.10).
- Traveling Salesman Problem (TSP) A combinatorial optimization problem in which an instance represents a collection of N points (cities) with specified distances (which may be geometric or nongeometric) between each pair, and a tour is defined as a path that visits each city exactly once and returns to its starting point. The goal is to find the shortest tour (introduction and section 6.1.1).
- Turing machine A simple universal computer, meaning that it is able to simulate the computation specified by any algorithm. A purely mathematical construct first described by Alan Turing in 1936, it consists of a tape divided into cells, each containing a symbol from some specified alphabet; a head that can read and write symbols and advance the tape one cell at a time; a finite table containing instructions for turning an input from the tape into an output; and a register that stores the current state of the machine (section 6.1.2).
- **Two-level system (TLS)** A degree of freedom or collection of degrees of freedom that can exist in one of two locally stable states; proposed to explain low-temperature thermal properties of glasses and other systems with quenched disorder (section 6.3.1).
- **Ultrametric space** A special type of metric space in which the triangle inequality is replaced by the *strong* triangle inequality. The result is that any three points in the space form the sides of an equilateral or acute isosceles triangle (section 5.6.3).
- Universality class Originally, a set of thermodynamic systems all of which display the same critical behavior at a second-order phase

transition, independent of microscopic details. Over the years the meaning has broadened to a less precise notion of a class of systems that display the same general behavior despite being very different in nature (section 6.4.1).

**Window** A fixed volume that is small compared to the system size, and in which correlation functions are (or should be) computed (section 7.1).

Zero-temperature dynamics See Noise-free dynamics.



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## INDEX

225-228, 248n2, 251n2 Anderson localization, 49-50, 245n9 Anfinsen, C.B., 163 annealing, 119, 245n7 simulated. See simulated annealing antiferromagnetism, 53, 59-60, 62, 67, 247n14, 248n7, 248n9 frustration and, 247n12 ground state, 59, 60f, 62 Arrhenius law, 150 AT line, 94 Austin, Robert, 151 Bennett, Charles, 230 Bloch, Felix, 49 Bloch wave, 49, 75 Boltzmann, Ludwig, 4 Boltzmann distribution, 36, 120, 188-189 Boltzmann factor, 36, 120, 188-189 Bray, Alan, 195 broken ergodicity, 88-89, 91

broken symmetry, 5, 26-31, 48,

Amit, D., 135-136

Anderson, Philip, 5, 49, 79,

127-129, 155, 169-170, 223,

241n18, 262n9 in complexity, 226–227 in crystal, 29–30 in ferro- and antiferromagnets, 59–60, 62 and ground states, 35 in spin glasses, 85–86, 98, 193–194. *See also* replica symmetry breaking Bryngelson, J.D., 163–164 Budnick, J.I., 65

Cannella, V., 65
cellular automata, 10, 232
Chaitin, Gregory, 229
chaos, 10, 170, 204–205
"disorder chaos," 210, 217
"edge of." *See under* complexity
"temperature chaos," 217
chaotic size dependence, 204–205, 217, 235, 236
combinatorial optimization, 3–4, 113–129
metastability and, 122 *NP*-completeness and, 114–117
phase transitions in, 129

combinatorial optimization	disorder:
(continued)	combinatorial optimization and,
rugged landscapes and, 122, 126	121
spin glasses and. See under spin	complexity and, 232, 235,
glasses	263n17
statistical mechanics and, 118-129	glasses and, 4, 7-8, 47-48, 69f
compactness, 258n11	proteins and, 153–159
complexity, 8–14, 218–238	quenched vs. thermal, 90–91
algorithmic, 11, 229-230	spin glasses and. See spin glasses, as
computational, 113–129	disordered systems
disorder and, 232, 235, 263n17	temperature and, 36–39, 55, 56f,
"edge of chaos" and, 10, 252n10,	57
262n11	vs. frustration, 12, 83
effective, 230–231	DLR equations, 258n14
emergence and, 6-7, 232-233	Dobrushin, Roland, 258n14
frustration and, 12, 233, 263n17	
general features of, 232-233	EA. See Edwards-Anderson
hierarchical organization and, 9,	Hamiltonian;
10, 12–13, 108, 223–225,	Edwards-Anderson order
234	parameter
measures of, 229-232	Edwards, Sam, 79
rugged landscapes and, 89,	Edwards-Anderson Hamiltonian,
172–173, 228, 232, 233	78–81, 91, 92, 178–181
spin glasses and. See spin glasses, as	Edwards-Anderson order parameter,
complex systems	85–86, 227
statistical, 231, 263n17	broken spin-flip symmetry and,
universality and, 231, 237, 263n21	85–86, 98, 193–194
condensed matter physics, 4–8, 16,	self-averaging and, 103, 105, 200,
222, 225–227	201
particle physics and, 16–17, 226,	emergence. See complexity,
241n18, 242n22, 244n39	emergence and; spin glasses,
Coyote, W.E., 150f	emergence and
Cragg, B.G., 131	energy barriers, 88
Crutchfield, James, 231, 262n14,	energy landscape, 74, 86–89, 110,
263n17	120, 122, 133
CSD. See chaotic size dependence	entropy, 5, 36–37, 94, 229, 244n2, 251n4
de Almeida, J.R.L., 93	disorder and, 38-39, 46-47,
Debye-Waller factor, 255n33	243n36
Derrida, Bernard, 138, 164, 172	in glasses, 45–47
Dirac, P.A.M., 61	Shannon, 11, 12, 229, 256n49

equilibrium, thermodynamic, 36,	in spin glasses, 12, 81-83, 110,
43–47, 71–72	233, 263n17
history-dependence and, 45,	vs. disorder, 12, 83
72–73	Fu, Yaotian, 127-129
observational timescale and, 44,	
47, 244n1	Gardner, Elizabeth, 138
ergodicity, 242n32	Garel, G., 256n45
broken, 88-89, 91	Gelatt, C.D., Jr., 119
translational, 260n28	Gell-Mann, Murray, 230
ergodic theorem, 250n25, 260n28,	"generalized rigidity," 5–7
260n30	Gibbs, J.W., 4
evolution, 9, 13, 228	Gibbs states. See thermodynamic
in immune response, 173–174	states
<i>NK</i> model and, 172–173	glass:
prebiotic, 168–170	as disordered system, 4, 7–8,
£ 52 57 50 (0 (2	47–48, 69f
ferromagnetism, 53, 57–59, 60, 62,	Kauzmann paradox, 46–47
97, 102, 103f, 248n7, 248n9	proteins and, 145, 154–159
droplet/scaling and, 196–197,	spin glasses and, 8, 69–70, 111
259n23	thermodynamic equilibrium and, 45–47
ground state, 57, 58f, 62, 69f	transition, 45–48, 245n4, 245n6.
mean field theory and, 215–216, 251n1	
	See also proteins, glass transition
mixed states in, 204, 258n16	in
neural networks and, 131	two-level systems in, 155 Goldanskii, Vitalii, 146, 156
Feynman, Richard, 242n30, 244n1 Fisher, Daniel, 195	Goldenfeld, N., 232
Frauenfelder, Hans, 146, 149	graph partitioning, 127–129
free energy, 38–39, 244n37, 244n38	graphs, 127–129
barriers, 88–89, 149–152, 154,	Grassberger, Peter, 231, 263n17
248n11	Griffith, J.S., 131
frustration and, 249n20	Gross, David, 256n44
landscape, 86–89, 165–167,	ground states, 34–35
248n11, 255n31	antiferromagnetic, 59, 60f, 62
self-averaging and, 104	boundary conditions and,
frustration, 12, 81–83, 249n20	182–187
in antiferromagnetism, 247n12	broken symmetry and, 35
combinatorial optimization and,	crystalline, 23f, 31, 32f, 35, 69f,
121–123	243n35
Mattis model and, 250n21	ferromagnetic, 57, 58f, 62, 69f
in proteins, 156–157, 163–165	infinite-volume, 180–187, 257n6
1	,, ,

ground states (continued) interfaces and, 187, 258n12 in spin glasses. See under spin glasses "windows" and, 185–187, 257n10	information retrieval and, 144 pattern recognition and, 144 phase transitions in, 136–138 protein structure prediction and, 167 "spin glass states" in, 135
Gurney, Kevin, 129	statistical mechanics of, 136–138
Gutfreund, H., 135	Hopfield net. See Hopfield model
	Huse, David, 195
Halperin, B.I., 155	
Hamilton, William Rowan, 25	immune response, 173–174
Hamiltonian:	spin glasses and, 174, 228
combinatorial optimization and, 118	Ising model, definition of, 79–80
crystal, 23–26	Kadanoff, L., 232
Heisenberg, 59–62, 247n19	Kauffman, Stuart, 170-172, 256n53
Hopfield model, 133–134	Kauzmann, Walter, 46
mean field, 91–92	Kirkpatrick, Scott, 92, 119, 123-125
NK model, 171–172	Kolmogorov, Andrey, 229
prebiotic evolution, 170	Kondo, Jun, 64
protein folding, 164	Kondo effect, 64–65
for protein structure prediction,	Krogh, A.S., 129
167–168	k-SAT, 129
randomly diluted ferromagnetic,	
128–129	Lanford, Oscar, III, 258n14
spin glass. See Edwards-Anderson	Levinthal, C., 162
Hamiltonian;	Little, W.A., 131
Sherrington-Kirkpatrick	Lloyd, Seth, 230
model, Hamiltonian	localization, 49-50, 245n9
Hebb, D.O., 131, 134	logical depth, 230, 234
Hebb rule, 131, 133-134	
Heisenberg, Werner, 61	magnetization, 55-57
Hertz, J.A., 129	as order parameter, 57, 59,
HIV, 174	247n14
Hodgkin-Huxley model, 254n24	self-averaging and, 104, 200
Hopfield, John, 131-132, 138, 141	Mattis model, 250n21, 253n16
Hopfield model, 131-138	may, be that as it, 218
associative memory and, 132-135	Maynard Smith, John, 256n52
capacity, 135-136, 137f	McCulloch, W.S., 130
dynamics,132-135	McCulloch-Pitts neuron, 130–131,
Hamiltonian, 133–134	133, 138, 141

McMillan, W.L., 195 mean field theory, 90–92 and dimensionality, 92, 251n1 of ordered systems, 215–216, 236, 251n1 of spin glasses. <i>See</i> replica symmetry breaking	networks, computation by neural networks, 129–144, 250n29. See also Hopfield model computation by, 129, 132–135, 138–144 as dynamical systems, 132–133, 141–144
Mertens, Stephan, 252n1	spin glasses and, 13, 131–144, 228
metastability. See under combinatorial optimization; proteins; spin glasses	NK model, 170–173  "complexity catastrophe" and, 256n53
metastates, 204-213, 236-237,	immune response and, 174
260n33	rugged landscapes in, 171-173
boundary conditions and, 210	spin glasses and, 171–172
chaotic dynamical systems and,	Noether, Emmy, 21
204–205, 211, 236–237	Noether's theorem, 21–22, 240n10
dispersal, 207–210, 211–212	NP-completeness, 114–117, 253n6
in droplet/scaling, 211	combinatorial optimization and,
invariance properties, 210	114–117
in replica symmetry breaking, 206–210	spin glasses and, 117, 253n7, 253n8
thermodynamic limit and,	statistical mechanics and, 117
205–206, 236–237	
Metropolis algorithm, 120-121, 136,	Onuchic, José, 166
253n10	order parameter:
Mézard, Marc, 256n44	antiferromagnetic, 59, 247n14
mixed states, 98, 190–191, 197–198,	broken symmetry and, 32-33
258n16, 258n17	of crystal, 34
decomposition into pure states,	ferromagnetic, 57
191–193, 197–198, 259n18,	of spin glasses. See
259n19	Edwards-Anderson order
in replica symmetry breaking,	parameter; replica symmetry
197–201, 203–204, 206–210	breaking
Monod, Jacques, 169	Orland, H., 256n45
Moore, Cristopher, 252n1	overlap:
Möore, Michael, 195	edge, 213
Mössbauer effect, 153, 248n8 Mydosh, J.A., 65	spin. <i>See under</i> replica symmetry breaking; pure states
Néel, Louis, 247n13	Pagels, Heinz, 230
neural computation. See neural	Palmer, Richard, 88, 129, 251n2

paramagnetism, 55, 56f, 57, 59, 67,	hydration shell, 149
97, 102, 136	levels of structure, 146
Parisi, Giorgio, 96	metastability in, 145, 165
Parisi order parameter. See under	myoglobin, 147–159
replica symmetry breaking	recombination kinetics, 146-153,
phase transitions, 5, 6, 39-41, 47,	157–158
188, 251n6, 254n21	rugged landscapes and, 160f,
antiferromagnetic, 59	165–167, 248n11, 255n31
in combinatorial optimization	slow relaxation in, 145, 149-152
problems, 129	spin glasses and, 13, 153–159,
dimensionality and, 83–84, 251n1	163–165, 228, 234, 256n45
ferromagnetic, 57–59	two-level systems in, 146,
in Hopfield model, 136–138	155–157
in spin glasses. See under spin	ultrametricity and, 159, 160f
glasses	pure states, 98, 188–193, 250n25,
Phillips, W.A., 155	258n17, 259n20
Pines, David, 228	in ferromagnetism, 197
Pitts, W., 130	in short-range spin glasses. See
Potts models, 256n43	under spin glasses
proteins, 144–168	spin overlaps and, 212
calmodulin, 159	
conformational dynamics,	quenching, 48, 119, 245n3, 245n7,
145–159	253n9
conformational substates, 147–159	
denaturation, 162, 256n41,	random energy model, 164, 172,
256n42	256n44
as disordered systems, 153–159	random field magnet, 206
folding, 13, 145, 146–148,	replica method, 95
159–168, 221; folding funnel,	replica symmetry breaking, 95–96,
165–167; free energy landscape	98–109, 213, 216, 234, 236,
in, 165–167; Levinthal paradox,	263n20
161–162, 165, 167, 255n40;	combinatorial optimization and,
molten globule phase, 165;	127
"principle of minimal	metastates and, 206–210
frustration," 163–165; rugged	non-self-averaging in, 101–105,
landscapes in, 165–167;	109, 199–203, 234
"thermodynamic hypothesis," 162–163	order parameters, 98–105, 109
	short-range spin glasses and, 110,
frustration and, 156–157, 163–165	194–195, 197–203, 206–210, 236–237
glass transition in, 154–159	spin overlaps in, 100–109, 194,
hemoglobin, 158f, 254n28	197–203, 206–211

thermodynamic states in, 98-109, 197–203, 206–210 ultrametricity in, 12-13, 108, 109, 209, 222, 224–225, 234, 252n16, 262n5, 262n6, 263n18 122, 126 RKKY interaction, 74-77 RNA world, 256n47 RSB. See replica symmetry breaking Ruelle, David, 258n14 rugged landscapes, 86, 88f, 89, 110, model 248n11 combinatorial optimization and, 122, 126 complex systems and, 89, 172–173, 228, 232, 233 immune response and, 173 in NK model, 171-173 in prebiotic evolution, 170 spin glasses: in proteins, 160f, 165-167, 248n11, 255n31 simulated annealing and, 119–120, 122, 126 in spin glasses, 12, 86-89, 110, 228, 233–234 216 Santa Fe Institute, 228, 239n3 Schrödinger, Erwin, 145, 254n27 Shalizi, C.R., 262n14

Santa Fe Institute, 228, 239n3
Schrödinger, Erwin, 145, 254n27
Shalizi, C.R., 262n14
Shannon, Claude, 229, 262n13
Shaw, G.L., 131
Sherrington, David, 92
Sherrington-Kirkpatrick model, 92–109, 175, 214–216, 234
broken symmetry in. *See* replica symmetry breaking
Hamiltonian, 92–93, 134, 139–140, 214–216, 225, 234
order parameters. *See under* replica symmetry breaking

phase transition in, 93-94, 176 Simon, Herbert, 223-225, 226, 234 simulated annealing, 119-126, 143 computer design and, 122-124 rugged landscapes and, 119-120, spin glasses and, 121-126, 234 Traveling Salesman problem and, 125, 126f SK. See Sherrington-Kirkpatrick Solomonoff, Ray, 229 Sompolinsky, H., 135 space translations, 18-20, 22, 26-29, 202-203, 241n20, 260n27 spin, quantum mechanical, 51-53, intrinsic magnetic moment and, 52 aging in, 13, 73, 249n12, 249n13 broken symmetry in, 85-86, 98, 193-194. See also replica symmetry breaking chaotic pairs scenario, 211-213, chaotic size dependence and, 204-205, 217, 235, 236 combinatorial optimization and, 1-4, 13, 112, 121-129, 234 as complex systems, 11-13, 89, 110-111, 218-219, 222, 224–225, 227–228, 233–238, 263n17 dilute magnetic alloys as, 64-66, 74 - 78"disorder chaos" in, 210, 217 as disordered systems, 1, 8, 12, 67, 68-71, 78, 79-81, 90-91, 110-111, 216, 233, 263n17 droplet/scaling scenario, 195-197,

213, 216, 260n32

313	2070
spin glasses (continued) emergence and, 6–7, 108, 111,	prebiotic evolution and, 13, 170, 228
225, 234, 238	proteins and, 13, 153–159,
frustration in, 12, 81–83, 110,	163–165, 228, 234, 256n45
233, 263n17	pure states in, 176, 193–216,
general properties of, 68	212–213, 251n9, 259n21, 261n40, 263n20
glasses and, 8, 69–70, 111 graphs and, 127–129	remanence behavior in, 72–73
ground states in, 69f, 82–83,	replica symmetry breaking and. See
177–187, 217, 257n7, 261n37	replica symmetry breaking
Hamiltonian. See	RKKY interaction and, 74–78
Edwards-Anderson Hamiltonian;	rugged landscapes and, 12, 86–89, 110, 228, 233–234
Sherrington-Kirkpatrick model,	simulated annealing and,
Hamiltonian	121–126, 234
immune response and, 174, 228	slow relaxation in, 13, 70–74, 234
insulators as, 74, 78	spatial ordering in, 67, 68-69,
k-SAT and, 129	85–86
magnetic susceptibility of, 65-68	specific heat of, 67-68, 250n23
mean field theory of. See	spin freezing in, 67–71, 85–86
Sherrington-Kirkpatrick model	stochastic stability and, 217, 235
metastability in, 12, 74, 87-89,	"temperature chaos" in, 217
110, 228, 233–234	thermodynamic equilibrium and,
metastates in. See metastates	70–71, 238
neural networks and, 13, 131–144,	"TNT" (trivial/nontrivial overlap)
228	scenario, 213, 216, 261n35
<i>NK</i> model and, 171–172	Traveling Salesman Problem and,
nonequilibrium dynamical	1–4, 129
behavior of, 13, 71–74,	ultrametricity and. See under
110–111, 234	ultrametricity
NP-completeness and, 117, 253n7, 253n8	spin overlap function. <i>See</i> replica symmetry breaking
order parameter. See	stochastic stability, 217, 235
Edwards-Anderson order	strange attractor, 204–205, 237
parameter	susceptibility, magnetic, 57–59,
overlaps. See under replica	246n11, 248n10
symmetry breaking	behavior at antiferromagnetic
phase transitions in, 83–86, 176,	phase transition, 59, 67
193–194. See also under	behavior at ferromagnetic phase
Sherrington-Kirkpatrick model	transition, 59
polymers and, 256n45	of spin glasses, 65–68

symmetry: broken. <i>See</i> broken symmetry conservation laws and, 21–22 in disordered systems, 202 of Hamiltonian, 26–29, 62, 202 in physics, 17–22, 24 permutation, 260n30 spin-flip, 85–86, 98, 178, 194, 250n26	Traveling Salesman Problem (TSP), 1–4, 113, 117, 118, 125–126, 129, 141–144 genome maps and, 239n2 graphs and, 128 Lin-Kernighan algorithm, 144f neural computation and, 141–144 spin glasses and, 1–4, 129 Turing machine, 115, 131, 253n4 Turing-computability, 262n15
Tank, D.W., 138, 141	two-level systems (TLS), 146,
Temperley, H.N.V., 131	155–157, 255n34
Theory of Everything, 262n8	in glasses, 155
thermodynamic depth, 230, 234	in proteins, 146, 155–157
thermodynamic limit, 188, 199, 205,	
236–237	ultrametric diffusion, 159, 160f,
thermodynamic states, 36,	262n6
97–98, 188–193, 206,	ultrametricity, 106–108
228, 236–237, 243n33, 258n15	in complexity, 9, 10, 12–13, 108, 223–225, 234
boundary conditions and, 189,	proteins and, 159, 160f
259n21, 261n34	in replica symmetry breaking. See
decomposition into pure states,	under replica symmetry breaking
191–193, 197–198, 259n18,	universality classes, 169
259n19	complexity and, 231, 237, 263n21
infinite-volume, 188–189	
mixed. See mixed states	van Hemmen, J.L., 253n16
pure. See pure states	Varma, C., 155
in replica symmetry breaking. See	Vecchi, M.P., 119
under replica symmetry breaking	
"windows" and, 189, 259n22	Weaver, Warren, 219-223, 226,
Thirumulai, H., 256n45	262n13
Thouless, David, 93, 251n2	Wiener, Norbert, 260n28
time reversal, 19, 21,	Wolynes, Peter, 163–164
240n3	
TLS. See two-level systems	Young, K., 231, 263n17