

Alexander Altland and Ben Simons

Condensed Matter Field Theory

SECOND EDITION

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Modern experimental developments in condensed matter and ultracold atom physics present formidable challenges to theorists. This book provides a pedagogical introduction to quantum field theory in many-particle physics, emphasizing the applicability of the formalism to concrete problems.

This second edition contains two new chapters developing path integral approaches to classical and quantum nonequilibrium phenomena. Other chapters cover a range of topics, from the introduction of many-body techniques and functional integration, to renormalization group methods, the theory of response functions, and topology. Conceptual aspects and formal methodology are emphasized, but the discussion focuses on practical experimental applications drawn largely from condensed matter physics and neighboring fields.

Extended and challenging problems with fully worked solutions provide a bridge between formal manipulations and research-oriented thinking. Aimed at elevating graduate students to a level where they can engage in independent research, this book complements courses on many particle theory.

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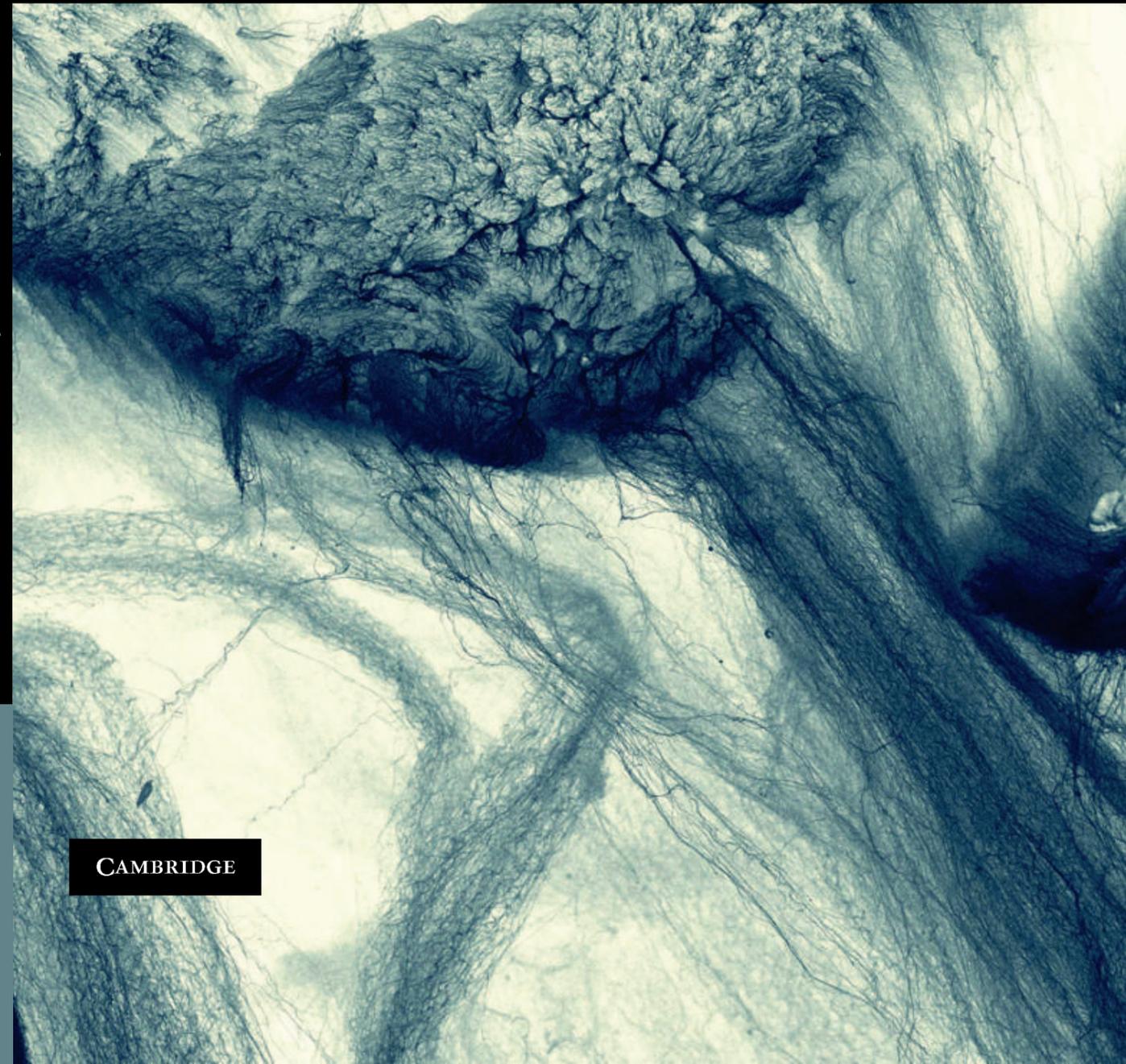


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Preface

In the past few decades, the field of quantum condensed matter physics has seen rapid and, at times, almost revolutionary development. Undoubtedly, the success of the field owes much to ground-breaking advances in experiment: already the controlled fabrication of phase coherent electron devices on the nanoscale is commonplace (if not yet routine), while the realization of ultra-cold atomic gases presents a new arena in which to explore strong interaction and condensation phenomena in Fermi and Bose systems. These, along with many other examples, have opened entirely new perspectives on the quantum physics of many-particle systems. Yet, important as it is, experimental progress alone does not, perhaps, fully explain the appeal of modern condensed matter physics. Indeed, in concert with these experimental developments, there has been a “quiet revolution” in condensed matter theory, which has seen phenomena in seemingly quite different systems united by common physical mechanisms. This relentless “unification” of condensed matter theory, which has drawn increasingly on the language of low-energy quantum field theory, betrays the astonishing degree of *universality*, not fully appreciated in the early literature.

On a truly microscopic level, all forms of quantum matter can be formulated as a many-body Hamiltonian encoding the fundamental interactions of the constituent particles. However, in contrast with many other areas of physics, in practically all cases of interest in condensed matter the structure of this operator conveys as much information about the properties of the system as, say, the knowledge of the basic chemical constituents tells us about the behavior of a living organism! Rather, in the condensed matter environment, it has been a long-standing tenet that the degrees of freedom relevant to the low-energy properties of a system are very often not the microscopic. Although, in earlier times, the passage between the microscopic degrees of freedom and the relevant low-energy degrees of freedom has remained more or less transparent, in recent years this situation has changed profoundly. It is a hallmark of many “deep” problems of modern condensed matter physics that the connection between the two levels involves complex and, at times, even controversial mappings. To understand why, it is helpful to place these ideas on a firmer footing.

Historically, the development of modern condensed matter physics has, to a large extent, hinged on the “unreasonable” success and “notorious” failures of *non-interacting* theories. The apparent impotency of interactions observed in a wide range of physical systems can be attributed to a deep and far-reaching principle of *adiabatic continuity*: the

quantum numbers that characterize a many-body system are determined by fundamental symmetries (translation, rotation, particle exchange, etc.). Providing that the integrity of the symmetries is maintained, the elementary “quasi-particle” excitations of an interacting system can be usually traced back “adiabatically” to those of the bare particle excitations present in the non-interacting system. Formally, one can say that the radius of convergence of perturbation theory extends beyond the region in which the perturbation is small. For example, this *quasi-particle correspondence*, embodied in Landau’s Fermi-liquid theory, has provided a reliable platform for the investigation of the wide range of Fermi systems from conventional metals to $^3\text{helium}$ fluids and cold atomic Fermi gases.

However, being contingent on symmetry, the principle of adiabatic continuity and, with it, the quasi-particle correspondence, must be abandoned at a *phase transition*. Here, interactions typically effect a substantial rearrangement of the many-body ground state. In the symmetry-broken phase, a system may – and frequently does – exhibit elementary excitations very different from those of the parent non-interacting phase. These elementary excitations may be classified as new species of quasi-particle with their own characteristic quantum numbers, or they may represent a new kind of excitation – a *collective mode* – engaging the cooperative motion of many bare particles. Many familiar examples fall into this category: when ions or electrons condense from a liquid into a solid phase, translational symmetry is broken and the elementary excitations – phonons – involve the motion of many individual bare particles. Less mundane, at certain field strengths, the effective low-energy degrees of freedom of a two-dimensional electron gas subject to a magnetic field (the quantum Hall system) appear as quasi-particles carrying a rational *fraction* (!) of the elementary electron charge – an effect manifestly non-perturbative in character.

This reorganization lends itself to a hierarchical perspective of condensed matter already familiar in the realm of particle physics. Each phase of matter is associated with a unique “non-interacting” reference state with its own characteristic quasi-particle excitations – a product only of the fundamental symmetries that classify the phase. While one stays within a given phase, one may draw on the principle of continuity to infer the influence of interactions. Yet this hierarchical picture delivers two profound implications. Firstly, within the quasi-particle framework, the underlying “bare” or elementary particles remain invisible (witness the fractionally charged quasi-particle excitations of the fractional quantum Hall fluid!). (To quote from P. W. Anderson’s now famous article “More is different,” (*Science* **177** (1972), 393–6), “the ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe.”) Secondly, while the capacity to conceive of new types of interaction is almost unbounded (arguably the most attractive feature of the condensed matter environment!), the freedom to identify non-interacting or free theories is strongly limited, constrained by the space of fundamental symmetries. When this is combined with the principle of continuity, the origin of the observed “universality” in condensed matter is revealed. Although the principles of adiabatic continuity, universality, and the importance of symmetries have been anticipated and emphasized long ago by visionary theorists, it is perhaps not until relatively recently that their mainstream consequences have become visible.

How can these concepts be embedded into a theoretical framework? At first sight, the many-body problem seems overwhelmingly daunting. In a typical system, there exist some 10^{23} particles interacting strongly with their neighbors. Monitoring the collective dynamics, even in a classical system, is evidently a hopeless enterprise. Yet, from our discussion above, it is clear that, by focussing on the coordinates of the collective degrees of freedom, one may develop a manageable theory involving only a restricted set of excitations. The success of quantum field theory in describing low-energy theories of particle physics as a successive hierarchy of broken symmetries makes its application in the present context quite natural. As well as presenting a convenient and efficient microscopic formulation of the many-body problem, the quantum field theory description provides a vehicle to systematically identify, isolate, and develop a low-energy theory of the collective field. Moreover, when cast as a field integral, the quantum field theory affords a classification of interacting systems into a small number of universality classes defined by their fundamental symmetries (a phenomenon not confined by the boundaries of condensed matter – many concepts originally developed in medium- or high-energy physics afford a seamless application in condensed matter). This phenomenon has triggered a massive trend of unification in modern theoretical physics. Indeed, by now, several sub-fields of theoretical physics have emerged (such as conformal field theory, random matrix theory, etc.) that define themselves not so much through any specific application as by a certain conceptual or methodological framework.

In deference to the importance attached to the subject, in recent years a number of texts have been written on the subject of quantum field theory within condensed matter. It is, therefore, pertinent for a reader to question the motivation for the present text. Firstly, the principal role of this text is as a primer aimed at elevating graduate students to a level where they can engage in independent research. Secondly, while the discussion of conceptual aspects takes priority over the exposure to the gamut of condensed matter applications, we have endeavored to keep the text firmly rooted in practical experimental application. Thirdly, as well as routine exercises, the present text includes extended problems which are designed to provide a bridge from formal manipulations to research-oriented thinking. Indeed, in this context, readers may note that some of the “answered” problems are deliberately designed to challenge: it is, after all, important to develop a certain degree of *intuitive* understanding of formal structures and, sadly, this can be acquired only by persistent and, at times, even frustrating training!

With this background, let us now discuss in more detail the organization of the text. To prepare for the discussion of field theory and functional integral techniques we begin in Chapter 1 by introducing the notion of a classical and a quantum field. Here we focus on the problem of lattice vibrations in the discrete harmonic chain, and its “ancestor” in the problem of classical and quantum electrodynamics. The development of field integral methods for the many-body system relies on the formulation of quantum mechanical theories in the framework of the second quantization. In Chapter 2 we present a formal and detailed introduction to the general methodology. To assimilate this technique, and motivate some of the examples discussed later in the text, a number of separate and substantial applications are explored in this chapter. In the first of these, we present (in second-quantized form) a somewhat cursory survey of the classification of metals and insulators, identifying a

canonical set of model Hamiltonians, some of which form source material for later chapters. In the case of the one-dimensional system, we will show how the spectrum of elementary collective excitations can be inferred using purely operator methods within the framework of the bosonization scheme. Finally, to close the chapter, we will discuss the application of the second quantization to the low-energy dynamics of quantum mechanical spin systems. As a final basic ingredient in the development of the quantum field theory, in Chapter 3 we introduce the Feynman path integral for the single-particle system. As well as representing a prototype for higher-dimensional field theories, the path integral method provides a valuable and recurring computational tool. This being so, we have included in this chapter a pedagogical discussion of a number of rich and instructive applications which range from the canonical example of a particle confined to a single or double quantum well, to the tunneling of extended objects (quantum fields), quantum dissipation, and the path integral formulation of spin.

Having accumulated all of the necessary background, in Chapter 4 we turn to the formulation and development of the field integral of the quantum many-particle system. Beginning with a discussion of coherent states for Fermi and Bose systems, we develop the many-body path integral from first principles. Although the emphasis in the present text is on the field integral formulation, the majority of early and seminal works in the many-body literature were developed in the framework of diagrammatic perturbation theory. To make contact with this important class of approximation schemes, in Chapter 5 we explore the way diagrammatic perturbation series expansions can be developed systematically from the field integral. Employing the ϕ^4 -theory as a canonical example, we describe how to explore the properties of a system in a high order of perturbation theory around a known reference state. To cement these ideas, we apply these techniques to the problem of the weakly interacting electron gas.

Although the field integral formulation provides a convenient means to organize perturbative approximation schemes as a diagrammatic series expansion, its real power lies in its ability to identify non-trivial reference ground states, or “mean-fields,” and to provide a framework in which low-energy theories of collective excitations can be developed. In Chapter 6, a fusion of perturbative and mean-field methods is used to develop analytical machinery powerful enough to address a spectrum of rich applications ranging from metallic magnetism and superconductivity to superfluidity. To bridge the gap between the (often abstract) formalism of the field integral, and the arena of practical application, it is necessary to infer the behavior of correlation functions. Beginning with a brief survey of concepts and techniques of experimental condensed matter physics, in Chapter 7 we highlight the importance of correlation functions and explore their connection with the theoretical formalism developed in previous chapters. In particular, we discuss how the response of many-body systems to various types of electromagnetic perturbation can be described in terms of correlation functions and how these functions can be computed by field theoretical means.

Although the field integral is usually simple to formulate, its properties are not always easy to uncover. Amongst the armory of tools available to the theorist, perhaps the most adaptable and versatile is the method of the renormalization group. Motivating

our discussion with two introductory examples drawn from a classical and a quantum theory, in Chapter 8 we become acquainted with the renormalization group method as a concept whereby nonlinear theories can be analyzed beyond the level of plain perturbation theory. With this background, we then proceed to discuss renormalization methods in more rigorous and general terms, introducing the notion of scaling, dimensional analysis, and the connection to the general theory of phase transitions and critical phenomena. To conclude this chapter, we visit a number of concrete implementations of the renormalization group scheme introduced and exemplified on a number of canonical applications.

In Chapter 9, we turn our attention to low-energy theories with non-trivial forms of long-range order. Specifically, we will learn how to detect and classify topologically non-trivial structures, and to understand their physical consequences. Specifically, we explore the impact of topological terms (i.e. θ -terms, Wess–Zumino terms, and Chern–Simons terms) on the behavior of low-energy field theories solely through the topology of the underlying field configurations. Applications discussed in this chapter include persistent currents, ’t Hooft’s θ -vacua, quantum spin chains, and the quantum Hall effects.

So far, our development of field theoretic methodologies has been tailored to the consideration of single-particle quantum systems, or many-body systems in thermal equilibrium. However, studies of classical nonequilibrium systems have a long and illustrious history, dating back to the earliest studies of thermodynamics, and these days include a range of applications from soft matter physics to population dynamics and ecology. At the same time, the control afforded by modern mesoscopic semiconducting and metallic devices, quantum optics, as well as ultracold atom physics now allow controlled access to quantum systems driven far from equilibrium. For such systems, traditional quantum field theoretical methodologies are inappropriate.

Starting with the foundations of non-equilibrium statistical mechanics, from simple one-step processes, to reaction–diffusion type systems, in Chapter 10 we begin by developing Langevin and Fokker–Planck theory, from which we establish classical Boltzmann transport equations. We then show how these techniques can be formulated in the language of the functional integral developing the Doi–Peliti and Martin–Siggia–Rose techniques. We conclude our discussion with applications to nonequilibrium phase transitions and driven lattice gases. These studies of the classical nonequilibrium system provide a platform to explore the quantum system. In Chapter 11, we develop the Keldysh approach to quantum non-equilibrium systems based, again, on the functional integral technique. In particular, we emphasize and exploit the close connections to classical nonequilibrium field theory, and present applications to problems from the arena of quantum transport.

To focus and limit our discussion, we have endeavored to distill material considered “essential” from the “merely interesting” or “background.” To formally acknowledge and identify this classification, we have frequently included reference to material which we believe may be of interest to the reader in placing the discussion in context, but which can be skipped without losing the essential thread of the text. These intermissions are signaled in the text as “Info” blocks.

At the end of each chapter, we have collected a number of pedagogical and instructive problems. In some cases, the problems expand on some aspect of the main text requiring only

an extension, or straightforward generalization, of a concept raised in the chapter. In other cases, the problems rather complement the main text, visiting fresh applications of the same qualitative material. Such problems take the form of case studies in which both the theory and the setting chart new territory. The latter provide a vehicle to introduce some core areas of physics not encountered in the main text, and allow the reader to assess the degree to which the ideas in the chapter have been assimilated. With both types of questions to make the problems more inclusive and useful as a reference, we have included (sometimes abridged, and sometimes lengthy) answers. In this context, Section 6.5 assumes a somewhat special role: the problem of phase coherent electron transport in weakly disordered media provides a number of profoundly important problems of great theoretical and practical significance. In preparing this section, it became apparent that the quantum disorder problem presents an ideal environment in which many of the theoretical concepts introduced in the previous chapters can be practiced and applied – to wit diagrammatic perturbation theory and series expansions, mean-field theory and collective mode expansions, correlation functions and linear response, and topology. We have therefore organized this material in the form of an extended problem set in Chapter 6.

This concludes our introduction to the text. Throughout, we have tried to limit the range of physical applications to examples which are rooted in experimental fact. We have resisted the temptation to venture into more speculative areas of theoretical condensed matter at the expense of excluding many modern and more-circumspect ideas which pervade the condensed matter literature. Moreover, since the applications are intended to help motivate and support the field theoretical techniques, their discussion is, at times, necessarily superficial. (For example, the hundreds pages of text in this volume could have been invested in their entirety in the subject of superconductivity!) Therefore, where appropriate, we have tried to direct interested readers to the more specialist literature.

In closing, we would like to express our gratitude to Jakob Müller-Hill, Tobias Micklitz, Jan Müller, Natalja Strelkova, Franjo-Frankopan Velic, Andrea Wolff, and Markus Zowislok for their invaluable assistance in the proofreading of the text. Moreover, we would also like to thank Julia Meyer for her help in drafting problems. Finally we would like to acknowledge Sasha Abanov for his advice and guidance in the drafting of the chapter on Topology.

As well as including additional material on the formulation of functional field integral methods to classical and quantum nonequilibrium physics in Chapters 10 and 11, in preparing the second edition of the text, we have endeavored to remove some of the typographical errors that crept into the first edition. Although it seems inevitable that some errors will still have escaped identification, it is clear that many many more would have been missed were it not for the vigilance of many friends and colleagues. In this context, we would particularly like to acknowledge the input of Piet Brouwer, Christoph Bruder, Chung-Pin Chou, Jan von Delft, Karin Everschor, Andrej Fischer, Alex Gezerlis, Sven Gnutzmann, Colin Kiegel, Tobias Lück, Patrick Neven, Achim Rosch, Max Schäfer, Matthias Sitte, Nobuhiko Taniguchi, and Matthias Vojta.

1

From particles to fields

To introduce some fundamental concepts of field theory, we begin by considering two simple model systems – a one-dimensional “caricature” of a solid, and a freely propagating electromagnetic wave. As well as exemplifying the transition from discrete to continuous degrees of freedom, these examples introduce the basic formalism of classical and quantum field theory, the notion of elementary excitations, collective modes, symmetries, and universality – concepts which will pervade the rest of the text.

One of the more remarkable facts about condensed matter physics is that phenomenology of fantastic complexity is born out of a Hamiltonian of comparative simplicity. Indeed, it is not difficult to construct microscopic “condensed matter Hamiltonians” of reasonable generality. For example, a prototypical metal or insulator might be described by the many-particle Hamiltonian, $H = H_e + H_i + H_{ei}$ where

$$\left. \begin{aligned} H_e &= \sum_i \frac{\mathbf{p}_i^2}{2m} + \sum_{i<j} V_{ee}(\mathbf{r}_i - \mathbf{r}_j), \\ H_i &= \sum_I \frac{\mathbf{P}_I^2}{2M} + \sum_{I<J} V_{ii}(\mathbf{R}_I - \mathbf{R}_J), \\ H_{ei} &= \sum_{iI} V_{ei}(\mathbf{R}_I - \mathbf{r}_i). \end{aligned} \right\} \quad (1.1)$$

Here, \mathbf{r}_i (\mathbf{R}_I) denote the coordinates of the valence electrons (ion cores) and H_e , H_i , and H_{ei} describe the dynamics of electrons, ions and the interaction of electrons and ions, respectively (see Fig. 1.1). Of course, the Hamiltonian Eq. (1.1) can be made “more realistic,” for example by remembering that electrons and ions carry spin, adding disorder, or introducing host lattices with multi-atomic unit-cells. However, for developing our present line of thought the prototype H will suffice.

The fact that a seemingly innocuous Hamiltonian like Eq. (1.1) is capable of generating the vast panopticon of metallic phenomenology can be read in reverse order: one will normally not be able to make theoretical progress by approaching the problem in an “*ab initio*” manner, i.e. by an approach that treats all microscopic constituents as equally relevant degrees of freedom.

How then can successful analytical approaches be developed? The answer to this question lies in a number of basic principles inherent in generic condensed matter systems.

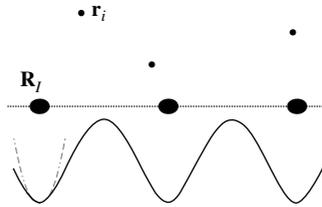


Figure 1.1 A one-dimensional cartoon of a (metallic) solid. Positively charged ions located at positions \mathbf{R}_I are surrounded by a conduction electron cloud (electron coordinates denoted by \mathbf{r}_i). While the motion of the ions is massively constrained by the lattice potential V_{ii} (indicated by the solid line and its harmonic approximation shown dashed), the dynamics of the electrons is affected by their mutual interaction (V_{ee}) and their interaction with the core ions (V_{ei}).

1. **Structural reducibility:** Not all components of the Hamiltonian (1.1) need to be treated simultaneously. For example, when the interest is foremost in the vibrational motion of the ion lattice, the dynamics of the electron system can often be neglected or, at least, be treated in a simplistic manner. Similarly, much of the character of the dynamics of the electrons is independent of the ion lattice, etc.
2. In the majority of condensed matter applications, one is interested not so much in the full profile of a given system, but rather in its energetically low-lying dynamics. This is motivated partly by practical aspects (in daily life, iron is normally encountered at room temperature and not at its melting point), and partly by the tendency of large systems to behave in a “universal” manner at low temperatures. Here **universality** implies that systems differing in microscopic detail (e.g. different types of interaction potentials, ion species, etc.) exhibit common collective behavior. As a physicist, one will normally seek for unifying principles in collective phenomena rather than to describe the peculiarities of individual species. However, universality is equally important in the *practice* of condensed matter theory. It implies, for example, that, at low temperatures, details of the functional form of microscopic interaction potentials are of secondary importance, i.e. that one may employ *simple* model Hamiltonians.
3. For most systems of interest, the number of degrees of freedom is formidably large with $N = \mathcal{O}(10^{23})$. However, contrary to first impressions, the magnitude of this figure is rather an advantage. The reason is that in addressing condensed matter problems we may make use of the **concepts of statistics** and that (precisely due to the largeness of N) statistical errors tend to be negligibly small.¹
4. Finally, condensed matter systems typically possess a number of intrinsic **symmetries**. For example, our prototype Hamiltonian above is invariant under simultaneous translation and rotation of all coordinates, which expresses the global Galilean invariance of the system (a continuous set of symmetries). Spin rotation invariance (continuous) and

¹ The importance of this point is illustrated by the empirical observation that the most challenging systems in physical sciences are of *medium* (and not large) scale, e.g., metallic clusters, medium-sized nuclei or large atoms consist of $\mathcal{O}(10^1\text{--}10^2)$ fundamental constituents. Such problems are well beyond the reach of few-body quantum mechanics while not yet accessible to reliable statistical modeling. Often the only viable path to approaching systems of this type is massive use of phenomenology.

time-reversal invariance (discrete) are other examples of frequently encountered symmetries. The general importance of symmetries cannot be over emphasized: symmetries entail the conservation laws that simplify any problem. Yet in condensed matter physics, symmetries are “even more” important. A conserved observable is generally tied to an energetically low-lying excitation. In the universal low-temperature regimes in which we will typically be interested, it is precisely the dynamics of these low-level excitations that governs the gross behavior of the system. In subsequent sections, the sequence “symmetry \mapsto conservation law \mapsto low-lying excitations” will be encountered time and again. At any rate, identification of the fundamental symmetries will typically be the first step in the analysis of a solid state system.

To understand how these basic principles can be used to formulate and explore “effective low-energy” field theories of solid state systems we will begin our discussion by focussing on the harmonic chain; a collection of atoms bound by a harmonic potential. In doing so, we will observe that the universal characteristics encapsulated by the low-energy dynamics² of large systems relate naturally to concepts of **field theory**.

1.1 Classical harmonic chain: phonons

Returning to the prototype Hamiltonian (1.1) discussed earlier, let us focus on the dynamical properties of the positively charged *core ions* that constitute the host lattice of a crystal. For the moment, let us neglect the fact that atoms are quantum objects and treat the ions as *classical* entities. To further simplify the problem, let us consider an atomic chain rather than a generic d -dimensional solid. In this case, the positions of the ions can be specified by a sequence of coordinates with an average lattice spacing a . Relying on the reduction principle (1) we will first argue that, to understand the behavior of the ions, the dynamics of the conduction electrons are of secondary importance, i.e. we will set $H_e = H_{ei} = 0$.

At strictly zero temperature, the system of ions will be frozen out, i.e. the one-dimensional ion coordinates $R_I \equiv \bar{R}_I = Ia$ settle into a regularly spaced array. Any deviation from a perfectly regular configuration has to be paid for by a price in potential energy. For low enough temperatures (principle 2), this energy will be approximately quadratic in the small deviation from the equilibrium position. The reduced low-energy **Hamiltonian** of our system then reads

$$H = \sum_{I=1}^N \left[\frac{P_I^2}{2M} + \frac{k_s}{2} (R_{I+1} - R_I - a)^2 \right], \quad (1.2)$$

where the coefficient k_s determines the steepness of the lattice potential. Notice that H can be interpreted as the Hamiltonian of N point-like particles of mass M elastically connected by springs with spring constant k_s (see Fig. 1.2).

² In this text, we will focus on the *dynamical* behavior of large systems, as opposed to their *static* structural properties. In particular, we will not address questions related to the formation of definite crystallographic structures in solid state systems.

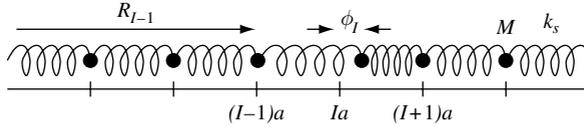


Figure 1.2 Toy model of a one-dimensional solid; a chain of elastically bound massive point particles.

Lagrangian formulation and equations of motion

What are the elementary low-energy excitations of the system? To answer this question we might, in principle, attempt to solve Hamilton's equations of motion. Indeed, since H is quadratic in all coordinates, such a program is, in this case, feasible. However, we must bear in mind that few of the problems encountered in general solid state physics enjoy this property. Further,

it seems unlikely that the low-energy dynamics of a macroscopically large chain – which we know from our experience will be governed by *large-scale* wave-like excitations – is adequately described in terms of an “atomistic” language; the relevant degrees of freedom will be of a different type. We should, rather, draw on the basic principles 1–4 set out above. Notably, we have so far paid attention neither to the intrinsic symmetry of the problem nor to the fact that N is large.

Crucially, to reduce a microscopic model to an effective low-energy theory, the Hamiltonian is often not a very convenient starting point. Usually, it is more efficient to start out from an *action*. In the present case, the **Lagrangian action** corresponding to a time interval $[0, t_0]$ is defined as $S = \int_0^{t_0} dt L(R, \dot{R})$, where $(R, \dot{R}) \equiv \{R_I, \dot{R}_I\}$ symbolically represents the set of all coordinates and their time derivatives. The **Lagrangian** L related to the Hamiltonian (1.2) is given by

$$L = T - U = \sum_{I=1}^N \left[\frac{M \dot{R}_I^2}{2} - \frac{k_s}{2} (R_{I+1} - R_I - a)^2 \right], \quad (1.3)$$

where T and U denote respectively the kinetic and potential energy.

Since we are interested in the properties of the large- N system, we can expect boundary effects to be negligible. This being so, we are at liberty to impose on our atomic chain the topology of a circle, i.e. we adopt periodic boundary conditions identifying $R_{N+1} = R_1$. Further, anticipating that the effect of lattice vibrations on the solid is weak (i.e. long-range atomic order is maintained) we may assume that the deviation of the ions from their

Joseph-Louis Lagrange 1736–1813

A mathematician who excelled in all fields of analysis, number theory, and celestial mechanics. In 1788 he published *Mécanique Analytique*, which summarised all the work done in the field of mechanics since the time of Newton, and is notable for its use of the theory of differential equations. In it he transformed mechanics into a branch of mathematical analysis.

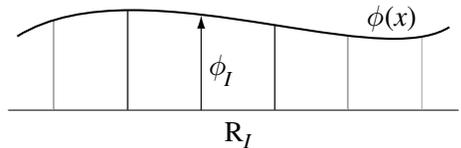


equilibrium position is small ($|R_I(t) - \bar{R}_I| \ll a$), and the integrity of the solid is maintained. With $R_I(t) = \bar{R}_I + \phi_I(t)$ ($\phi_{N+1} = \phi_1$) the Lagrangian (1.3) assumes the simplified form

$$L = \sum_{I=1}^N \left[\frac{M}{2} \dot{\phi}_I^2 - \frac{k_s}{2} (\phi_{I+1} - \phi_I)^2 \right].$$

To make further progress, we will now make use of the fact that we are not concerned with the behavior of our system on “atomic” scales. (In any case, for such purposes a modeling like the one above would be much too primitive!) Rather, we are interested in experimentally observable behavior that manifests itself on macroscopic length scales (principle 2). For example, one might wish to study the specific heat of the solid in the limit of infinitely many atoms (or at least a macroscopically large number, $\mathcal{O}(10^{23})$). Under these conditions, microscopic models can usually be substantially simplified (principle 3). In particular, it is often permissible to subject a discrete lattice model to a so-called **continuum limit**, i.e. to neglect the discreteness of the microscopic entities and to describe the system in terms of effective continuum degrees of freedom.

In the present case, taking a continuum limit amounts to describing the lattice fluctuations ϕ_I in terms of smooth functions of a continuous variable x (see the figure where the [horizontal] displacement of the point particles has been plotted along the vertical). Clearly such a description makes sense only if relative fluctuations on atomic scales are weak (for otherwise the smoothness condition would be violated). However, if this condition is met – as it will be for sufficiently large values of the stiffness constant k_s – the continuum description is much more powerful than the discrete encoding in terms of the “vector” $\{\phi_I\}$. All steps that we will need to take to go from the Lagrangian to concrete physical predictions will be much easier to formulate.



Introducing continuum degrees of freedom $\phi(x)$, and applying a first-order Taylor expansion,³ let us define

$$\phi_I \rightarrow a^{1/2} \phi(x) \Big|_{x=Ia}, \quad \phi_{I+1} - \phi_I \rightarrow a^{3/2} \partial_x \phi(x) \Big|_{x=Ia}, \quad \sum_{I=1}^N \rightarrow \frac{1}{a} \int_0^L dx,$$

where $L = Na$. Note that, as defined, the functions $\phi(x, t)$ have dimensionality $[\text{length}]^{1/2}$. Expressed in terms of the new degrees of freedom, the continuum limit of the Lagrangian then reads

$$L[\phi] = \int_0^L dx \mathcal{L}(\phi, \partial_x \phi, \dot{\phi}), \quad \mathcal{L}(\phi, \partial_x \phi, \dot{\phi}) = \frac{m}{2} \dot{\phi}^2 - \frac{k_s a^2}{2} (\partial_x \phi)^2, \quad (1.4)$$

³ Indeed, for reasons that will become clear, higher-order contributions to the Taylor expansion are immaterial in the long-range continuum limit.