Cambridge University Press
978-0-521-76975-4 - Condensed Matter Field Theory, Second Edition
Alexander Altland and Ben Simons
Excerpt
More information

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, $H = H_\mathrm{e} + H_\mathrm{i} + H_\mathrm{ei}$ where

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

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.

Cambridge University Press
978-0-521-76975-4 - Condensed Matter Field Theory, Second Edition
Alexander Altland and Ben Simons
Excerpt
More information

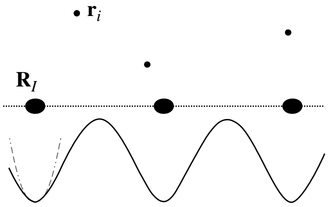


Figure 1.1 A one-dimensional cartoon of a (metallic) solid. Positively charged ions located at positions $\mathbf{R}_I$ are surrounded by a conduction electron cloud (electron coordinates denoted by $\mathbf{r}_i$). While the motion of the ions is massively constrained by the lattice potential $V_{\rm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

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.

CAMBRIDGE

Cambridge University Press
978-0-521-76975-4 - Condensed Matter Field Theory, Second Edition
Alexander Altland and Ben Simons
Excerpt
More information

> 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 dynamics[2] 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 $H_{\mathrm{e}} = H_{\mathrm{ei}} = 0$.

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

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

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.

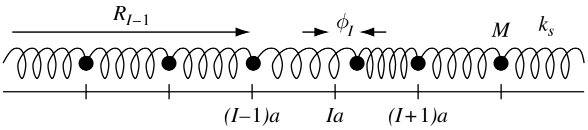


Figure 1.2 Toy model of a one-dimensional solid; a chain of elastically bound massive point particles.

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.

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.

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

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

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

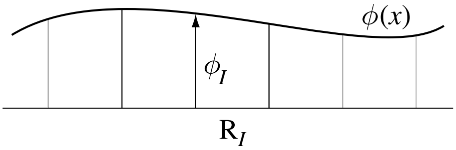
Since we are interested in the properties of the large-N system, we can expect boundary effects to be negligible. This being so, we are at liberty to impose on our atomic chain the topology of a circle, i.e. we adopt periodic boundary conditions identifying $R_{N+1} = R_1$. Further, anticipating that 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

Cambridge University Press
978-0-521-76975-4 - Condensed Matter Field Theory, Second Edition
Alexander Altland and Ben Simons
Excerpt
More information

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

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

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

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

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

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

---

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

Cambridge University Press
978-0-521-76975-4 - Condensed Matter Field Theory, Second Edition
Alexander Altland and Ben Simons
Excerpt
More information

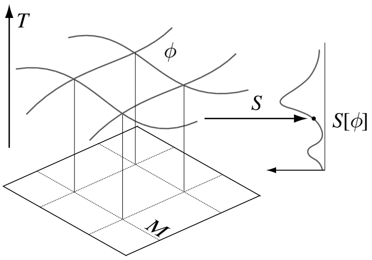


Figure 1.3 Schematic visualization of a field: a mapping ϕ from a base manifold M into a target space T (in this case, T are the real numbers; but, in general, T can be more complicated). A functional assigns to each ϕ a real number $S[\phi]$. The grid embedded into M indicates that fields in condensed matter physics arise as continuum limits of discrete mappings.

where the **Lagrangian density** $\mathcal{L}$ has dimensionality [energy]/[length] and we have designated the particle mass by the more common symbol $m \equiv M$. Similarly, the classical action assumes the continuum form

$$\boxed{S[\phi] = \int dt\; L[\phi] = \int dt \int_0^L dx\; \mathcal{L}(\phi, \partial_x\phi, \dot{\phi}).} \tag{1.5}$$

We have thus succeeded in abandoning the N-point particle description in favor of one involving *continuous* degrees of freedom, a **(classical) field**. The dynamics of the latter are specified by the **functionals** L and S, which represent the continuum generalizations of the discrete classical Lagrangian and action, respectively.

> INFO The continuum variable ϕ is our first encounter with a **field**. Before proceeding with our example, let us pause to make some preliminary remarks on the general definition of these objects. This will help to place the subsequent discussion of the atomic chain into a broader context. Formally, a field is a smooth mapping
>
> $$\begin{aligned}\phi: \quad M &\to T,\\ z &\mapsto \phi(z),\end{aligned}$$
>
> from a certain manifold M,[4] often called the "base manifold," into a "target" or "field manifold" T (see Fig. 1.3).[5] In our present example, $M = [0, L] \times [0, t] \subset \mathbb{R}^2$ is the product of intervals in space and time, and $T = \mathbb{R}$. In fact, the factorization $M \subset \mathcal{R} \times \mathcal{T}$ into a space-like manifold $\mathcal{R}$ multiplied by a one-dimensional time-like manifold $\mathcal{T}$ is inherent in most applications of condensed matter physics.[6]

---

[4] If you are unfamiliar with the notion of manifolds (for a crash course, see page 537), think of M and T as subsets of some vector space. For the moment, this limitation won't do any harm.

[5] In some (rare) cases it becomes necessary to define fields in a more general sense (e.g. as sections of mathematical objects known as fiber bundles). However, in practically all condensed matter applications the more restrictive definition above will suffice.

[6] By contrast, the condition of Lorentz invariance implies the absence of such factorizations in relativistic field theory. In classical statistical field theories, i.e. theories probing the thermodynamic behavior of large systems, M is just space-like.

Cambridge University Press
978-0-521-76975-4 - Condensed Matter Field Theory, Second Edition
Alexander Altland and Ben Simons
Excerpt
More information

However, the individual factors $\mathcal{R}$ and $\mathcal{T}$ may, of course, be more complex than in our prototypical problem above. As to the target manifold, not much can be said in general; depending on the application, the realizations of T range from real or complex numbers over vector spaces and groups to the "fanciest objects" of mathematical physics.

In applied field theory, fields appear not as final objects but rather as input to *functionals* (see Fig. 1.3). Mathematically, a functional $S : \phi \mapsto S[\phi] \in \mathbb{R}$ is a mapping that takes a field as its argument and maps it into the real numbers. The functional profile $S[\phi]$ essentially determines the character of a field theory. Notice that the argument of a functional is commonly indicated in square brackets [ ].

While these formulations may appear unnecessarily abstract, remembering the mathematical backbone of the theory often helps to avoid confusion. At any rate, it takes some time and practice to get used to the concept of fields and functionals. Conceptual difficulties in handling these objects can be overcome by remembering that any field in condensed matter physics arises as the limit of a *discrete* mapping. In the present example, the field $\phi(x)$ is obtained as a continuum approximation of the discrete vector $\{\phi_I\} \in \mathbb{R}^N$; the functional $L[\phi]$ is the continuum limit of the function $L : \mathbb{R}^N \to \mathbb{R}$, etc. While in practical calculations fields are usually easier to handle than their discrete analogs, it is sometimes helpful to think about problems of field theory in a discrete language. Within the discrete picture, the mathematical apparatus of field theory reduces to finite-dimensional calculus.

Although Eq. (1.4) contains the full information about the model, we have not yet learned much about its actual behavior. To extract concrete physical information from Eq. (1.4) we need to derive **equations of motion**. At first sight, it may not be entirely clear what is meant by the term "equations of motion" in the context of an infinite-dimensional model: the equations of motion relevant for the present problem are obtained as the generalization of the conventional Lagrange equations of N-particle classical mechanics to a model with infinitely many degrees of freedom. To derive these equations we need to generalize Hamilton's extremal principle (i.e. the route from an action to the associated equations of motion) to infinite dimensions. As a warm-up, let us briefly recapitulate how the extremal principle works for a system with one degree of freedom.

Suppose the dynamics of a classical *point* particle with coordinate $x(t)$ is described by the classical Lagrangian $L(x, \dot{x})$, and action $S[x] = \int dt\, L(x, \dot{x})$. **Hamilton's extremal principle** states that the configurations $x(t)$ that are *actually realized* are those that extremize the action, $\delta S[x] = 0$. This means (for a substantiated discussion, see Section 1.2 below) that, for any smooth curve $t \mapsto y(t)$,

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon}(S[x + \epsilon y] - S[x]) = 0. \tag{1.6}$$

To first order in ϵ, the action has to remain invariant. Applying this condition, one finds that it is fulfilled if and only if x satisfies **Lagrange's equation of motion**

$$\boxed{\frac{d}{dt}(\partial_{\dot{x}} L) - \partial_x L = 0.} \tag{1.7}$$

EXERCISE Recapitulate the derivation of (1.7) from the classical action.

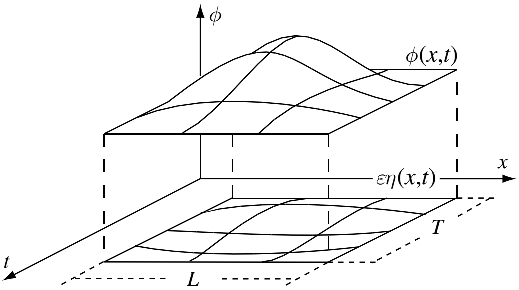


Figure 1.4 Schematic showing the variation of the field associated with the action functional. Notice that the variation $\epsilon\eta$ is supposed to vanish on the boundaries of the base $M = [0, L] \times [0, t]$.

In Eq. (1.5) we are dealing with a system of infinitely many degrees of freedom, $\phi(x, t)$. Yet Hamilton's principle is general and we may see what happens if Eq. (1.5) is subjected to an extremal principle analogous to Eq. (1.6). To do so, we substitute $\phi(x, t) \to \phi(x, t) + \epsilon\eta(x, t)$ into Eq. (1.5) and require vanishing of the first-order contribution to an expansion in ϵ (see Fig. 1.4). When applied to the specific Lagrangian (1.4), substituting the "varied" field leads to

$$S[\phi + \epsilon\eta] = S[\phi] + \epsilon \int dt \int_0^L dx \left(m\dot{\phi}\dot{\eta} - k_{\mathrm{s}} a^2 \partial_x \phi \partial_x \eta \right) + \mathcal{O}(\epsilon^2).$$

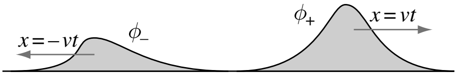
Integrating by parts and requiring that the contribution linear in ϵ vanishes, one obtains

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(S[\phi + \epsilon\eta] - S[\phi] \right) = -\int dt \int_0^L dx \left(m\ddot{\phi} - k_{\mathrm{s}} a^2 \partial_x^2 \phi \right) \eta \overset{!}{=} 0.$$

(Notice that the boundary terms vanish identically.) Now, since η was defined to be an arbitrary smooth function, the integral above can vanish only if the factor in parentheses is globally vanishing. Thus the equation of motion takes the form of a **wave equation**

$$\boxed{\left(m\partial_t^2 - k_{\mathrm{s}} a^2 \partial_x^2 \right) \phi = 0.} \tag{1.8}$$

The solutions of Eq. (1.8) have the general form $\phi_+(x - vt) + \phi_-(x + vt)$ where $v = a\sqrt{k_{\mathrm{s}}/m}$, and $\phi_\pm$ are arbitrary smooth functions of the argument. From this we can deduce that the basic low-energy **elementary excitations** of our model are lattice vibrations propagating as **sound waves** to the left or right at a constant velocity v (see the figure).[7] The trivial behavior of our model is of course a direct consequence of its simplistic definition – no dissipation, dispersion, or other non-trivial ingredients. Adding these refinements leads to the general classical theory of lattice vibrations (such as that described in the text by Ashcroft and Mermin[8]). Finally, notice that



---

[7] Strictly speaking, the modeling of our system enforces a periodicity constraint $\phi_\pm(x + L) = \phi_\pm(x)$. However, in the limit of a large system, this aspect becomes inessential.

[8] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Holt–Saunders International, 1983).

Cambridge University Press
978-0-521-76975-4 - Condensed Matter Field Theory, Second Edition
Alexander Altland and Ben Simons
Excerpt
More information

the elementary excitations of the chain have little in common with its "microscopic" constituents (the atomic oscillators). Rather they are **collective excitations**, i.e. elementary excitations comprising a macroscopically large number of microscopic degrees of freedom.

INFO The "relevant" **excitations of a condensed matter system** can, but need not, be of collective type. For example, the interacting electron gas (a system to be discussed in detail below) supports microscopic excitations – charged quasi-particles standing in 1:1 correspondence with the electrons of the original microscopic system – while the collective excitations are plasmon modes of large wavelength and engaging many electrons. Typically, the nature of the fundamental excitations cannot be straightforwardly inferred from the microscopic definition of a model. Indeed, the mere *identification* of the relevant excitations often represents the most important step in the solution of a condensed matter problem.

Hamiltonian formulation

Sir William Rowan Hamilton 1805–65
A mathematician credited with the discovery of quaternions, the first non-commutative algebra to be studied. He also invented important new methods in mechanics. (Image from W. R. Hamilton, *Collected Papers*, vol. II, Cambridge University Press, 1940.

An important characteristic of any excitation is its *energy*. How much energy is stored in the sound waves of the harmonic chain? To address this question, we need to switch back to a Hamiltonian formulation. Once again, this is achieved by generalizing standard manipulations from point mechanics to the continuum. Remembering that, for a Lagrangian of a point particle, $p \equiv \partial_{\dot{x}} L$ is the momentum conjugate to the coordinate x, let us consider the Lagrangian *density* and define[9]

$$\boxed{\pi(x) \equiv \frac{\partial \mathcal{L}(\phi, \partial_x \phi, \dot{\phi})}{\partial \dot{\phi}(x)},} \tag{1.9}$$

as the **canonical momentum** associated with ϕ (at the point x). In common with ϕ, the momentum π is a continuum degree of freedom. At each space point it may take an independent value. Notice that $\pi(x)$ is nothing but the continuum generalization of the lattice momentum P_I of Eq. (1.2). (Applied to P_I, a continuum approximation like $\phi_I \to \phi(x)$ would produce $\pi(x)$.) The **Hamiltonian density** is then defined as usual through the Legendre transformation,

$$\boxed{\mathcal{H}(\phi, \partial_x \phi, \pi) = \left(\pi\dot{\phi} - \mathcal{L}(\phi, \partial_x\phi, \dot{\phi})\right)\Big|_{\dot{\phi}=\dot{\phi}(\phi,\pi)},} \tag{1.10}$$

---

[9] In field theory literature it is popular to denote the momentum by a Greek letter.

from where the full Hamiltonian is obtained as $H = \int_0^L dx\, \mathcal{H}$.

EXERCISE Verify that the transition $L \to H$ is a straightforward continuum generalization of the Legendre transformation of the N-particle Lagrangian $L(\{\phi_I\}, \{\dot{\phi}_I\})$.

Having introduced a Hamiltonian, we are in a position to determine the energy of the sound waves. Application of Eq. (1.9) and (1.10) to the Lagrangian of the atomic chain yields $\pi(x,t) = m\dot{\phi}(x,t)$ and

$$H[\pi, \phi] = \int dx \left(\frac{\pi^2}{2m} + \frac{k_s a^2}{2} (\partial_x \phi)^2 \right). \tag{1.11}$$

Considering, say, a right-moving sound-wave excitation, $\phi(x,t) = \phi_+(x - vt)$, we find that $\pi(x,t) = -mv\partial_x\phi_+(x-vt)$ and $H[\pi,\phi] = k_s a^2 \int dx [\partial_x \phi_+(x-vt)]^2 = k_s a^2 \int dx\ [\partial_x\phi_+(x)]^2$, i.e. a positive definite, time-independent expression, as one would expect.

Before proceeding, let us note an interesting feature of the energy functional: in the limit of an infinitely shallow excitation, $\partial_x \phi_+ \to 0$, the energy vanishes. This sets the stage for the last of the principles (4) hitherto unconsidered, **symmetry**. The Hamiltonian of an atomic chain is invariant under simultaneous translation of all atom coordinates by a fixed increment: $\phi_I \to \phi_I + \delta$, where δ is constant. This expresses the fact that a global translation of the solid as a whole does not affect the internal energy. Now, the ground state of any specific realization of the solid will be defined through a static array of atoms, each located at a fixed coordinate $R_I = Ia \Rightarrow \phi_I = 0$. We say that the translational symmetry is "spontaneously broken," i.e. the solid has to decide where exactly it wants to rest. However, spontaneous breakdown of a symmetry does not imply that the symmetry disappeared. On the contrary, infinite-wavelength deviations from the pre-assigned ground state come close to global translations of (macroscopically large portions of) the solid and, therefore, cost a vanishingly small amount of energy. This is the reason for the vanishing of the sound wave energy in the limit $\partial_x \phi \to 0$. It is also our first encounter with the aforementioned phenomenon that symmetries lead to the formation of soft, i.e. low-energy, excitations. A much more systematic exposition of these connections will be given in Chapter 6.

Ludwig Boltzmann 1844–1906
A physicist whose greatest achievement was in the development of statistical mechanics, which explains and predicts how the properties of atoms (such as mass, charge, and structure) determine the visible properties of matter (such as viscosity, thermal conductivity, and diffusion).

To conclude our discussion of the classical harmonic chain, let us consider the **specific heat**, a quantity directly accessible in experiment. A rough estimate of this quantity can be readily obtained from the microscopic harmonic Hamiltonian (1.2). According to the principles of statistical mechanics, the thermodynamic energy density is given by

$$u = \frac{1}{L} \frac{\int d\Gamma\ e^{-\beta H} H}{\int d\Gamma\ e^{-\beta H}} = -\frac{1}{L} \partial_\beta \ln \int d\Gamma\ e^{-\beta H},$$

where $\beta = 1/k_B T$, $\mathcal{Z} \equiv \int d\Gamma e^{-\beta H}$ is the **Boltzmann partition function** and the phase space volume element $d\Gamma = \prod_{I=1}^N dR_I dP_I$. We will set $k_B = 1$ throughout. The specific heat