Chapter 1

From Particles to Fields

The goal of this section is to introduce the machinery of classical and quantum field theory in the framework of a simple model of lattice dynamics. In doing so, we will become acquainted with the notion of elementary excitations, collective modes, and universality — concepts which will pervade the rest of the course.

1.1 Free Scalar Field Theory: Phonons

As a grossly simplified model of a (one-dimensional) quantum solid consider a chain of point particles of mass m (atoms) which are elastically connected by springs with spring constant k_s (chemical bonds) (see Fig. 1.1). The aim of this chapter will be to construct

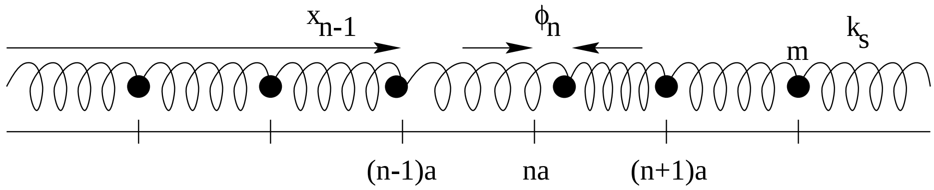


Figure 1.1: Toy model of a one-dimensional solid: A chain of elastically bound massive point particles.

an effective quantum field theory of the vibrations of the one-dimensional solid. However, before doing so, we will first consider its classical behaviour. Analysing the classical case will not only tell us how to quantise the system, but also get us acquainted with some basic methodological concepts of field theory in general.

1.1.1 Classical Chain

The classical **Lagrangian**[1] of the N-atom chain is given by

$$L = T - V = \sum_{n=1}^{N} \left(\frac{m}{2}\dot{x}_n^2 - \frac{k_s}{2}(x_{n+1} - x_n - a)^2 \right), \tag{1.1}$$

where the first term accounts for the kinetic energy of the particles whilst the second describes their coupling.[2] For convenience, we adopt periodic boundary conditions such that $x_{N+1} = Na + x_1$. Anticipating that the effect of lattice vibrations on the solid is weak (i.e. long-range atomic order is maintained) we will assume that (a) the n-th atom has its equilibrium position at $\bar{x}_n \equiv na$ (with a the mean inter-atomic distance), and (b) that the deviation from the equilibrium position is small ($|x_n(t) - \bar{x}_n| \ll a$), i.e. the integrity of the solid is maintained. With $x_n(t) = \bar{x}_n + \phi_n(t)$ ($\phi_{N+1} = \phi_1$) the Lagrangian (1.1) takes the form

$$L = \sum_{n=1}^{N} \left(\frac{m}{2}\dot{\phi}_n^2 - \frac{k_s}{2}\left(\phi_{n+1} - \phi_n\right)^2 \right).$$

Typically, one is not concerned with the behaviour of a given system on 'atomic' scales. (In any case, for such purposes, a modelling like the one above would be much too primitive!) Rather, one is interested in **universal** features, i.e. experimentally observable behaviour that manifests itself on macroscopic length scales. 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. 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 of the system and to describe it in terms of effective continuum degrees of freedom.

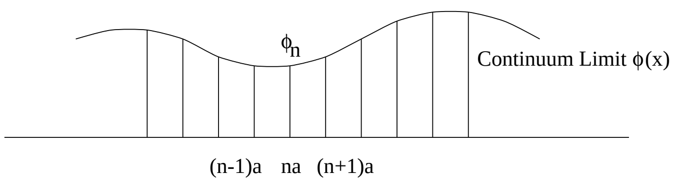
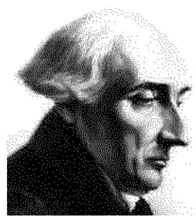


Figure 1.2: Continuum limit of the harmonic chain.

[1] 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.



[2] In realistic solids, the inter-atomic potential is, of course, more complex than just quadratic. Yet, for "weak coupling", the quadratic contribution plays a dominant role. For the sake of simplicity we, therefore, neglect the effects caused by higher order contributions.

In the present case, taking a continuum limit amounts to describing the lattice fluctuations ϕ_n in terms of *smooth functions* of a continuous variable x (Fig. 1.2). Clearly such a description makes sense only if relative fluctuations on atomic scales are weak (for otherwise the smoothness condition would be violated). Introducing continuum degrees of freedom $\phi(x)$, and applying a first order Taylor expansion,[3] we define

$$\phi_n \to a^{1/2}\phi(x)\Big|_{x=na}, \qquad \phi_{n+1} - \phi_n \to a^{3/2}\partial_x\phi(x)\Big|_{x=na}, \qquad \sum_{n=1}^{N} \longrightarrow \frac{1}{a}\int_0^L dx,$$

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

$$L[\phi] = \int_0^L dx\; \mathcal{L}(\phi, \partial_x\phi, \dot{\phi}), \qquad \mathcal{L}(\phi, \partial_x\phi, \dot{\phi}) = \frac{m}{2}\dot{\phi}^2 - \frac{k_s a^2}{2}(\partial_x\phi)^2, \tag{1.2}$$

where the **Lagrangian density** $\mathcal{L}$ has dimensionality [energy]/[length]. (Here, and throughout, we will adopt the shorthand convention $\dot{O} \equiv \partial_t O$.) The **classical action** associated with the dynamics of a certain configuration ϕ is defined as

$$\boxed{S[\phi] = \int dt\; L[\phi] = \int dt \int_0^L dx\; \mathcal{L}(\phi, \partial_x\phi, \dot{\phi})} \tag{1.3}$$

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

▷ INFO. In the physics literature, mappings of functions into the real or complex numbers are generally called **functionals**. The argument of a functional is commonly indicated in angular brackets [.]. E.g., in this case, S maps the 'functions' $\partial_x\phi(x,t)$ and $\dot{\phi}(x,t)$ to the real number $S[\phi]$.

Although Eq. (1.2) contains the full information about the model, we have not yet learned much about its actual behaviour. To extract concrete physical information from (1.2) 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 answer to this question lies in Hamilton's[4] extremal principle of classical mechanics:

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

[4] Sir William Rowan Hamilton 1805-1865: A mathematician credited with the discovery of quaternions, the first non-commutative algebra to be studied. He also invented important new methods in Mechanics.

Suppose that 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 realised* are those that extremise the action, viz. $\delta S[x] = 0$. This means that for any smooth curve $y(t)$,

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon}(S[x + \epsilon y] - S[x]) = 0, \tag{1.4}$$

i.e. 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 solves **Lagrange's equation of motion** (a revision exercise)

$$\boxed{\frac{d}{dt}(\partial_{\dot{x}} L) - \partial_x L = 0} \tag{1.5}$$

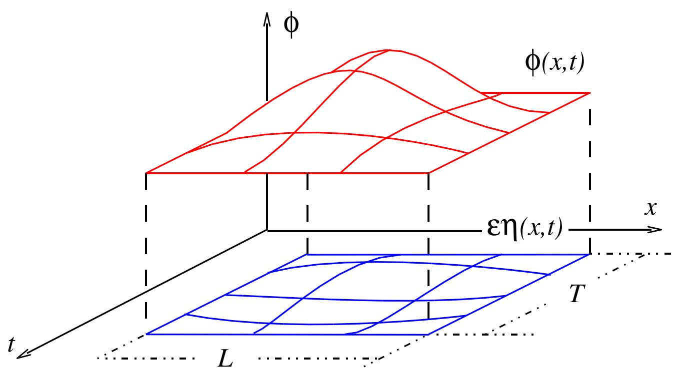


Figure 1.3: Schematic diagram showing the variation of the field associated with the action functional.

In Eq. (1.3) 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 (1.3) is subjected to an extremal principle analogous to Eq. (1.4). To do so, we substitute

$$\phi(x, t) \to \phi(x, t) + \epsilon\eta(x, t)$$

into Eq. (1.3) and demand vanishing of the first order contribution to an expansion in ϵ (see Fig. 1.3). When applied to the specific Lagrangian (1.2), substituting the 'varied' field leads to

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

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

$$\int dt \int dx \left(m\ddot{\phi} - k_s a^2 \partial_x^2 \phi \right) \eta = 0.$$

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

$$\boxed{\left(m\partial_t^2 - k_s a^2 \partial_x^2\right)\phi = 0} \tag{1.6}$$

The solutions of Eq. (1.6) have the general form $\phi_+(x+vt) + \phi_-(x-vt)$ where $v = a\sqrt{k_s/m}$, 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 Fig. 1.4). The trivial behaviour 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 (see, e.g., Ref. [2]).

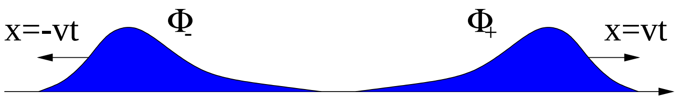


Figure 1.4: Visualisation of the fundamental left and right moving excitations of the classical harmonic chain.

▷ INFO. **Functional Analysis**: before proceeding, let us briefly digress and revisit the derivation of the equations of motion (1.6). Although straightforward, the calculation was neither efficient, nor did it reveal general structures. In fact, what we did — expanding explicitly to first order in the variational parameter ϵ — had the same status as evaluating derivatives by explicitly taking limits: $f'(x) = \lim_{\epsilon\to 0}(f(x+\epsilon) - f(x))/\epsilon$. Moreover, the derivation made explicit use of the particular form of the Lagrangian, thereby being of limited use with regard to a general understanding of the construction scheme. Given the importance attached to extremal principles in all of field theory, it is worthwhile investing some effort in constructing a more efficient scheme for general variational analysis of continuum theories. In order to carry out this programme we first need to introduce a mathematical tool of functional analysis, viz. the concept of functional differentiation.

In working with functionals, one is often concerned with how a given functional behaves under (small) variations of its argument function. In order to understand how answers to these types of questions can be systematically found, it is helpful to temporarily return to a discrete way of thinking, i.e. to interpret the argument f of a functional $F[f]$ as the limit $N \to \infty$ of a discrete vector $\mathbf{f} = \{f_n \equiv f(x_n), n = 1, \ldots N\}$, where $\{x_n\}$ denotes a discretisation of the support of $\mathbf{f}$ (cf. Fig. 1.2 $\phi \leftrightarrow f$). Prior to taking the continuum limit, $N \to \infty$, $\mathbf{f}$ has the status of a N-dimensional vector and $F[\mathbf{f}]$ is a function defined over N-dimensional space. After the continuum limit, $\mathbf{f}$ becomes a function itself and $F[\mathbf{f}]$ becomes a functional.

Now, within the discrete picture it is clear how the variational behaviour of functions is to be analysed, e.g. the condition that for all ϵ and all vectors $\mathbf{g}$, the linear expansion of $F[\mathbf{f}+\epsilon\mathbf{g}]$ ought to vanish, is simply to say that the total derivative, $\nabla F[\mathbf{f}]$, at $\mathbf{f}$ has to be zero. In practice, one often expresses conditions of this type in terms of a certain basis. For example, in a Cartesian basis of N unit vectors, $\hat{\mathbf{e}}_n$, $n = 1, \ldots, N$,

$$F[\mathbf{f}+\epsilon\mathbf{g}] = F[\mathbf{f}] + \epsilon\sum_{n=1}^{N}(\partial_{f_n}F[\mathbf{f}])g_n + \cdots, \qquad \partial_{f_n}F[\mathbf{f}] \equiv \lim_{\epsilon\to 0}\frac{1}{\epsilon}\left(F[\mathbf{f}+\epsilon\hat{\mathbf{e}}_n] - F[\mathbf{f}]\right). \tag{1.7}$$

The total derivative of F is zero, if and only if $\forall n$, $\partial_{f_n} F = 0$.

Taking the continuum limit of such identities will lead us to the concept of **functional differentiation**, a central tool in all areas of field theory. In the continuum limit, sums running from 1 to N become integrals. The nth unit vector $\hat{\mathbf{e}}_n$ becomes a function that is everywhere vanishing save at one point where it equals ∞, i.e. $\epsilon\hat{\mathbf{e}}_n \to \delta_x$, where the function $\delta_x(y) \equiv \delta(x-y)$.[5] Thus, the continuum limit of Eq. (1.7) reads

$$\begin{aligned} F[f+\epsilon g] &= F[f] + \epsilon \int dx \frac{\delta F[f]}{\delta f(x)} g(x) + \mathcal{O}(\epsilon^2) \\ \frac{\delta F[f]}{\delta f(x)} &\equiv \lim_{\epsilon \to 0} \frac{1}{\epsilon} \left(F[f+\epsilon \delta_x] - F[f] \right). \end{aligned} \tag{1.8}$$

Here the second line represents the definition of the functional derivative, i.e. the generalisation of a conventional partial derivative to infinitely many dimensions. Experience shows that it takes some time to get used to the concept of functional differentiation. However, after some practice it will become clear that this operation is not only extremely useful but also as easy to handle as conventional partial differentiation. In particular, all rules known from ordinary calculus (product-rule, chain-rule, etc.) immediately generalise to the functional case (as follows straightforwardly from the way the functional derivative has been introduced). For example, the generalisation of the standard chain rule,

$$\partial_{f_n} F[\mathbf{g}[\mathbf{f}]] = \sum_m \partial_{g_m} F[\mathbf{g}] \Big|_{\mathbf{g}=\mathbf{g}[\mathbf{f}]} \partial_{f_n} g_m[\mathbf{f}]$$

reads

$$\frac{\delta F[g[f]]}{\delta f(x)} = \int dy \left. \frac{\delta F[g]}{\delta g(y)} \right|_{g=g[f]} \frac{\delta g(y)[f]}{\delta f(x)}. \tag{1.9}$$

Furthermore, given some functional $F[f]$, we can Taylor expand it as

$$F[f] = F[0] + \int dx_1 \frac{\delta F[f]}{\delta f(x_1)} f(x_1) + \int dx_1 \int dx_2 \; \frac{1}{2} \frac{\delta^2 F[f]}{\delta f(x_2) \delta f(x_1)} f(x_1) f(x_2) + \cdots$$

Some basic definitions underlying functional differentiation as well as their finite dimensional counterparts are summarised in the following table:

entity	discrete	continuum
f	vector	function
$F[f]$	multi-dimensional function	functional
Cartesian basis	$\hat{\mathbf{e}}_n$	δ_x
‘partial derivative’	$\partial_{f_n} F[\mathbf{f}]$	$\frac{\delta F[f]}{\delta f(x)}$

[5] If you find the singularity of the continuum version of the unit-vector difficult to accept, remember that the limit

$$\sum_n \langle \hat{\mathbf{e}}_n | \mathbf{f} \rangle = f_n \to \int dy \; \delta_x(y) f(y) = f(x)$$

enforces $\delta_x(y) = \delta(x-y)$.

After this preparation, let us re-examine the extremal condition for a general action $S[x]$ by means of functional differentiation. As follows from the definition of the functional derivative (1.7), the action is extremal, if and only if $\forall x(t)$,

$$\frac{\delta S[x]}{\delta x(t)} = \int dt' \frac{\delta L(x(t'), \dot{x}(t'))}{\delta x(t)} = 0.$$

Employing the definition of the action in terms of the Lagrangian and applying the chain rule (1.9), we find

$$\int dt' \frac{\delta L(x(t'), \dot{x}(t'))}{\delta x(t)} = \int dt' \Big[\frac{\partial L(x(t'), \dot{x}(t'))}{\partial x(t')} \overbrace{\frac{\partial x(t')}{\partial x(t)}}^{\delta(t'-t)} + \frac{\partial L(x(t'), \dot{x}(t'))}{\partial \dot{x}(t')} \overbrace{\frac{\partial \dot{x}(t')}{\partial x(t)}}^{d_{t'}\delta(t'-t)} \Big],$$

From this result a rearrangement by integration obtains the familiar Euler-Lagrange equations

$$\frac{\delta S[x]}{\delta x(t)} = \frac{\partial L}{\partial x(t)} - \frac{d}{dt} \frac{\partial L}{\partial \dot{x}(t)} = 0.$$

It is left as a straightforward exercise to show that the general equations of motion of a classical continuum system with Lagrangian density $\mathcal{L}(\phi, \partial_x \phi, \dot{\phi})$ is given by

$$\boxed{\frac{\delta S[\phi]}{\delta \phi(x,t)} = \frac{\partial \mathcal{L}}{\partial \phi} - \frac{d}{dt} \frac{\partial \mathcal{L}}{\partial \dot{\phi}} - \frac{d}{dx} \frac{\partial \mathcal{L}}{\partial(\partial_x \phi)}} \tag{1.10}$$

Eq. (1.10) represents the generalisation of Lagrange's equation of motion of point mechanics to classical field theory (1.5). The particular application to the equations of motion of the simple phonon model (1.2) are illustrative of a *general principle.* All field theoretical models — be they classical or quantum — are represented in terms of certain actions whose extremal field configurations play a fundamental role.

$\triangleright$ EXERCISE. Write down the equation of motion corresponding to the Lagrangian density $\mathcal{L} = \mathcal{L}(\phi, \partial_x^2 \phi, \dot{\phi})$.

After this digression, let us return to the discussion of the original model (1.2). As mentioned above, the classical vibrational physics of solids can be formulated in terms of models like Eq. (1.2) and its generalisations. On the other hand it is known (e.g. from the experimental study of specific heat [2]) that various aspects of the physics of lattices are non-classical and necessitate a quantum mechanical description. Hence, what is called for is an extension of the classical field theory to a quantum field theory.

1.1.2 Quantum Chain

The first question to ask is a conceptual one: how can a model like (1.2) be quantised in general? As a matter of fact there exists a standard procedure of quantising Lagrangian continuum theories which closely resembles the quantisation of point mechanics. The first step is to introduce canonical momenta conjugate to the continuum degrees of freedom (coordinates) ϕ which will later be used to introduce canonical commutation relations. The natural generalisation of the definition $p_n \equiv \partial_{\dot{x}_n} L$ of point mechanics to a continuum suggests

$$\boxed{\pi(x) \equiv \frac{\partial \mathcal{L}(\phi, \partial_x \phi, \dot{\phi})}{\partial \dot{\phi}(x)}} \tag{1.11}$$

or, more concisely, $\pi = \partial_{\dot{\phi}} \mathcal{L}$. In common with ϕ, the **canonical momentum** π is a continuum degree of freedom. At each space point it may take an independent value. From the Lagrangian, we can define the Hamiltonian,

$$\boxed{H[\phi, \pi] \equiv \int dx\ \mathcal{H}(\phi(x), \pi(x)), \qquad \mathcal{H}(\phi, \pi) \equiv \pi \dot{\phi} - \mathcal{L}(\phi, \partial_x \phi, \dot{\phi})}$$

where $\mathcal{H}$ represents the **Hamiltonian density**. (All the quantities appearing in $\mathcal{H}$ are to be expressed in terms of π and ϕ.) In particular, applied to the lattice model (1.2),

$$\mathcal{H}(\phi, \pi) = \frac{1}{2m}\pi^2 + \frac{k_s a^2}{2}(\partial_x \phi)^2.$$

where $\pi = m\dot{\phi}$.

In this form, the Hamiltonian can be quantised according to the rules: (i) promote $\phi(x)$ and $\pi(x)$ to operators: $\phi \mapsto \hat{\phi}$, $\pi \mapsto \hat{\pi}$, and (ii) generalise the canonical commutation relations of one particle quantum mechanics, $[\hat{p}_m, \hat{x}_n] = -i\hbar\delta_{mn}$ according to[6]

$$\boxed{[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x - x')} \tag{1.12}$$

Operator-valued functions like $\hat{\phi}$ and $\hat{\pi}$ are generally referred to as **quantum fields**. Employing these definitions, we obtain the quantum Hamiltonian density

$$\hat{\mathcal{H}}(\hat{\phi}, \hat{\pi}) = \frac{1}{2m}\hat{\pi}^2 + \frac{k_s a^2}{2}(\partial_x \hat{\phi})^2. \tag{1.13}$$

The Hamiltonian above represents a quantum field theoretical *formulation* of the problem but not yet a *solution*. In fact, the development of a spectrum of methods for the analysis of quantum field theoretical models will represent a major part of this lecture course. At this point the objective is merely to exemplify how physical information can be extracted from models like (1.13).

As with any function, operator-valued functions can be represented in a variety of different ways. In particular they can be subjected to Fourier transform,

$$\left\{ \begin{array}{l} \hat{\phi}_k \\ \hat{\pi}_k \end{array} \right. \equiv \frac{1}{L^{1/2}} \int_0^L dx\ e^{\{\mp ikx} \left\{ \begin{array}{l} \hat{\phi}(x) \\ \hat{\pi}(x) \end{array} \right., \qquad \left\{ \begin{array}{l} \hat{\phi}(x) \\ \hat{\pi}(x) \end{array} \right. = \frac{1}{L^{1/2}} \sum_k e^{\{\pm ikx} \left\{ \begin{array}{l} \hat{\phi}_k \\ \hat{\pi}_k \end{array} \right., \tag{1.14}$$

[6]Note that the dimensionality of both the quantum and classical continuum fields is compatible with the dimensionality of the Dirac δ-function, $[\delta(x - x')] = [\text{Length}]^{-1}$.

where $\sum_k$ represents the sum over all Fourier coefficients indexed by quantised coordinates or "momenta" $k = 2\pi m/L$, $m \in \mathcal{Z}$. (Do not confuse the momenta k with the 'operator momentum' $\hat{\pi}$!) Note that the *real* classical field $\phi(x)$ quantises to an *Hermitian* quantum field $\hat{\phi}(x)$ implying that $\hat{\phi}_k = \hat{\phi}^\dagger_{-k}$ (and similarly for $\hat{\pi}_k$) — exercise. In the Fourier representation, the transformed field operators obey the canonical commutation relations (exercise)

$$\boxed{[\hat{\pi}_k, \hat{\phi}_{k'}] = -i\hbar\delta_{kk'}}$$

When expressed in the Fourier representation, making use of the identity

$$\int dx\ (\partial\hat{\phi})^2 = \sum_{k,k'}(ik\hat{\phi}_k)(ik'\hat{\phi}_{k'})\overbrace{\frac{1}{L}\int_0^L dx e^{i(k+k')x}}^{\delta_{k+k',0}} = \sum_k k^2\hat{\phi}_k\hat{\phi}_{-k}\left(\equiv \sum_k k^2|\hat{\phi}_k|^2\right)$$

together with a similar relation for $\int dx\ \hat{\pi}^2$, the Hamiltonian assumes the "near diagonal" form[7]

$$\hat{H} = \sum_k \left[\frac{1}{2m}\hat{\pi}_k\hat{\pi}_{-k} + \frac{k_s a^2}{2}k^2\hat{\phi}_k\hat{\phi}_{-k}\right]. \tag{1.15}$$

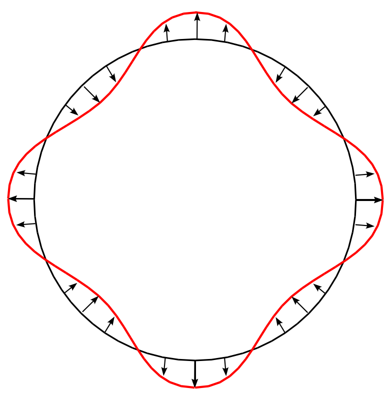


Figure 1.5: Coarse visualisation of the quantised phonon field. Each of the modes $\hat{\phi}_k$ is governed by a harmonic oscillator Hamiltonian that depends parametrically on the momentum k. Right: Linear dispersion relation characteristic of acoustic phonons.

In this form, the Hamiltonian can be identified as nothing more than a superposition of independent **harmonic oscillators**.[8] This result is actually not difficult to understand

[7] As a point of notation, when expressed in terms of a complete orthonormal basis $|m\rangle$, a general Hamiltonian can be expressed as a matrix, $H_{mn} = \langle m|\hat{H}|n\rangle$. In the eigenbasis $|\alpha\rangle$, the Hamiltonian is said to be diagonalised, viz. $H_{\alpha\beta} = \langle\alpha|\hat{H}|\beta\rangle = E_\alpha\delta_{\alpha\beta}$. In the present case, when expressed in the Fourier basis, the matrix elements correlate only k with $-k$.

[8] The only difference between (1.15) and the canonical form of an oscillator Hamiltonian $\hat{H} = \hat{p}^2/(2m)+ m\omega^2\hat{x}^2/2$ is the presence of the sub-indices k and $-k$ (a consequence of $\hat{\phi}^\dagger_k = \hat{\phi}_{-k}$). As we will show shortly, this difference is inessential.

(see Fig. 1.5): Classically, the system supports a discrete set of wave excitations, each indexed by a wave number $k = 2\pi m/L$. (In fact, we could have performed a Fourier transformation of the *classical* fields $\phi(x)$ and $\pi(x)$ to represent the Hamiltonian function as a superposition of classical harmonic oscillators.) Within the quantum picture, each of these excitations is described by an oscillator Hamiltonian operator with a k-dependent frequency. However, it is important not to confuse the atomic constituents, also oscillators (albethey coupled), with the independent *collective* oscillator modes described by $\hat{H}$.

The description above, albeit perfectly valid, still suffers from a deficiency: Our analysis amounts to explicitly describing the effective low energy excitations of the system (the waves) in terms of their microscopic constituents (the atoms). Indeed the different contributions to $\hat{H}$ keeps track of details of the microscopic oscillator dynamics of individual k-modes. However, it would be much more desirable to develop a picture where the relevant excitations of the system, the waves, appear as fundamental units, without explicit account of underlying microscopic details. (As with hydrodynamics, information is encoded in terms of collective density variables rather than through individual molecules.) As preparation for the construction of this improved formulation of the system, let us temporarily focus on a single oscillator mode.

1.1.3 Revision of the Quantum Harmonic Oscillator

Consider a standard harmonic oscillator (HO) Hamiltonian

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 \,.$$

The few first energy levels $\epsilon_n = \hbar\omega\left(n + \frac{1}{2}\right)$ and the associated Hermite polynomial eigenfunctions are displayed schematically in Fig. 1.6.

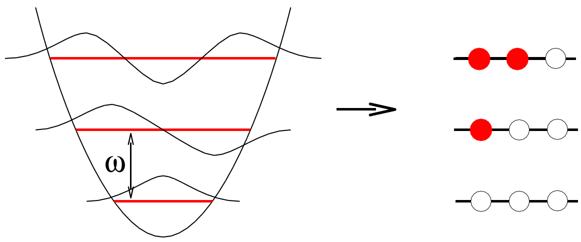


Figure 1.6: Low lying energy levels/states of the harmonic oscillator Hamiltonian.

In quantum mechanics, the HO has, of course, the status of a single-particle problem. However, the fact that the energy levels are *equidistant* suggests an alternative interpretation: One can think of a given energy state ϵ_n as an accumulation of n elementary entities, or **quasi-particles**, each having energy $\hbar\omega$. What can be said about the features of these new objects? First, they are structureless, i.e. the only 'quantum number' identifying the quasi-particles is their energy $\hbar\omega$ (otherwise n-particle states formed of the quasi-particles would not be equidistant). This implies that the quasi-particles must be *bosons*. (The same state $\hbar\omega$ can be occupied by more than one particle, see Fig. 1.6.)

This idea can be formulated in quantitative terms by employing the formalism of ladder-operators in which the operators $\hat{p}$ and $\hat{x}$ are traded for the pair of Hermitian adjoint operators $\hat{a} \equiv \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p})$, $\hat{a}^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p})$. Up to a factor of i, the transformation $(\hat{x}, \hat{p}) \to (\hat{a}, \hat{a}^\dagger)$ is canonical, i.e. the new operators obey the canonical commutation relation

$$[\hat{a}, \hat{a}^\dagger] = 1\,. \tag{1.16}$$

More importantly, the a-representation of the Hamiltonian is very simple, viz.

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right), \tag{1.17}$$

as can be checked by direct substitution. Suppose now, we had been given a zero eigenvalue state $|0\rangle$ of the operator $\hat{a}$: $\hat{a}|0\rangle = 0$. As a direct consequence, $\hat{H}|0\rangle = (\hbar\omega/2)|0\rangle$, i.e. $|0\rangle$ is identified as the ground state of the oscillator.[9] The complete hierarchy of higher energy states can now be generated by setting $|n\rangle \equiv (n!)^{-1/2}\,(\hat{a}^\dagger)^n|0\rangle$.

▷ Exercise. Using the canonical commutation relation, verify that $\hat{H}|n\rangle = \hbar\omega(n+1/2)|n\rangle$ and $\langle n|n\rangle = 1$.

So far, we have succeeded merely in finding yet another way of constructing eigenstates of the quantum HO problem. However, the 'real' advantage of the a-representation is that it naturally affords a many-particle interpretation. Temporarily forgetting about the original definition of the oscillator, let us *declare* $|0\rangle$ to represent a 'vacuum' state, i.e. a state with zero particles present. Next, imagine that $\hat{a}^\dagger|0\rangle$ is a state with a single featureless particle (the operator $\hat{a}^\dagger$ does not carry any quantum number labels) of energy $\hbar\omega$. Similarly, $(\hat{a}^\dagger)^n|0\rangle$ is considered as a many-body state with n particles, i.e. within the new picture, $\hat{a}^\dagger$ is an operator that creates particles. The total energy of these states is given by $\hbar\omega \times$ (occupation number). Indeed, it is straightforward to verify that $\hat{a}^\dagger\hat{a}|n\rangle = n|n\rangle$, i.e. the Hamiltonian basically counts the number of particles. While, at first sight, this may look unfamiliar, the new interpretation is internally consistent. Moreover, it achieves what we had asked for above, i.e. it allows an interpretation of the excited states of the HO as a superposition of independent structureless entities.

▷ Info. The representation above illustrates the capacity to think about individual quantum problems in **complementary pictures**. This principle finds innumerable applications in modern condensed matter physics. To get used to it one has to realize that the existence of different interpretations of a given system is by no means heretic but, rather, is consistent with the spirit of quantum mechanics. Indeed, it is one of the prime principles of quantum theories that there is no such thing as 'the real system' which underpins the phenomenology. The only thing that matters is observable phenomena. For example, we will see later that the 'fictitious' quasi-particle states of oscillator systems *behave* as 'real' particles, i.e. they have dynamics, can interact, be detected experimentally, etc. From a quantum point of view there is actually no fundamental difference between these objects and the 'real' particles.

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[9]... as can be verified by explicit construction: Switching to a real space representation, the solution of the equation $[x + \hbar\partial_x/(m\omega)]\langle x|0\rangle = 0$ obtains the familiar ground state wave function $\langle x|0\rangle = \sqrt{2\pi\hbar/(m\omega)}e^{-m\omega x^2/2\hbar}$.

1.1.4 Quasi-Particle Interpretation of the Quantum Chain

Returning to the oscillator chain, one can transform the Hamiltonian (1.15) to a form analogous to (1.17) by defining the ladder operators[10]

$$\hat{a}_k \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_k + i\frac{1}{m\omega_k}\hat{\pi}_{-k}\right), \qquad \hat{a}_k^\dagger \equiv \sqrt{\frac{m\omega_k}{2\hbar}}\left(\hat{\phi}_{-k} - i\frac{1}{m\omega_k}\hat{\pi}_k\right),$$

where $\omega_k = v|k|$, and $v = a(k_s/m)^{1/2}$ denotes the classical sound wave velocity. With this definition, applying the commutation relations, one finds that the ladder operators obey the commutation relations (characteristic of Bose particles)

$$\begin{aligned} [a_k, a_{k'}^\dagger] &= \frac{i}{2\hbar}\Big(\overbrace{[\hat{\pi}_{-k}, \hat{\phi}_{-k'}]}^{-i\hbar\delta_{kk'}} - [\hat{\phi}_k, \hat{\pi}_{k'}]\Big) = \delta_{kk'}, \\ [a_k, a_{k'}] &= \frac{i}{2\hbar}\left([\hat{\pi}_{-k}, \hat{\phi}_{k'}] + [\hat{\phi}_k, \hat{\pi}_{-k'}]\right) = 0, \qquad [a_k^\dagger, a_{k'}^\dagger] = 0. \end{aligned} \tag{1.18}$$

With this definition, one finds that the Hamiltonian assumes the diagonal form

$$\boxed{\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right)} \tag{1.19}$$

Equations (1.18) and (1.19) represent the final result of our analysis: The Hamiltonian $\hat{H}$ takes the form of a sum a set of harmonic oscillators with characteristic frequencies ω_k. In the limit $k \to 0$ (i.e. long wavelength), one finds $\omega_k \to 0$; excitations with this property are said to be **massless**.

An excited state of the system is indexed by a set $\{n_k\} = (n_1, n_2, \ldots)$ of quasi-particles with energy $\{\omega_k\}$. Physically, the quasi-particles of the harmonic chain are identified with the **phonon modes** of the solid. A comparison with measured phonon spectra (Fig. 1.7) reveals that, at low momenta, $\omega_k \sim |k|$ in agreement with our simplistic model (even in spite of the fact that the spectrum was recorded for a three-dimensional solid with non-trivial unit cell — universality!).

1.2 †Quantum Electrodynamics (QED)

▷ Additional Example: As a second and important example of an analogous quantum field theory, consider electrodynamics. In this lecture course quantum electrodynamics (QED) will play comparatively little role. Nonetheless it is worthwhile to mention it briefly because

- ▷ QED is historically the oldest and still most successful field theory. (The QED result for the anomalous magnetic moment of the electron agrees with experiment up to a precision of $\mathcal{O}(10^{-6})$!)

[10] As for the consistency of these definitions, recall that $\hat{\phi}_k^\dagger = \hat{\phi}_{-k}$ and $\hat{\pi}_k^\dagger = \hat{\pi}_{-k}$. Under these conditions the second of the definitions below indeed follows from the first upon taking the Hermitian adjoint.

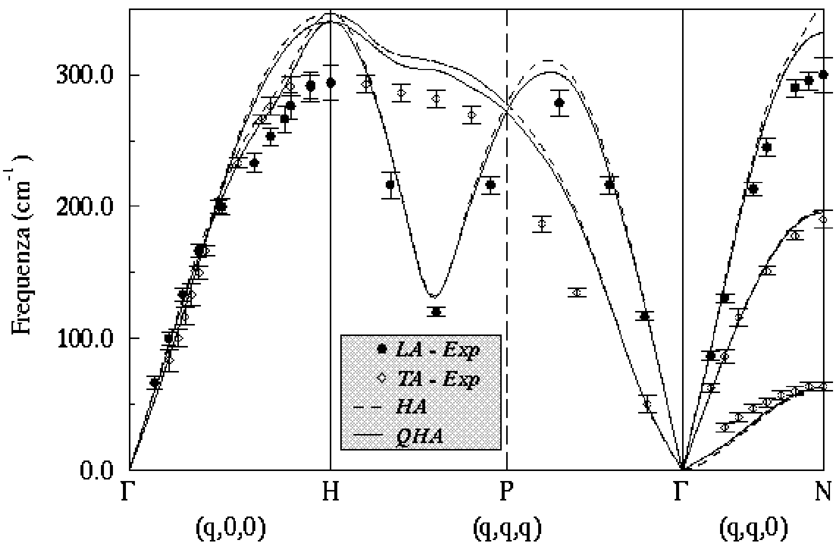


Figure 1.7: Typical phonon spectra of a crystal with a BCC lattice. The data is sensitive to both longitudinal (LA) and transverse (TA) acoustic phonons. Notice that for small momenta, the dispersion is linear.

▷ Quantised electromagnetic fields (→ photons) play a significant role in many areas of condensed matter physics.

In the following short discussion we merely wish to illustrate the basic *principle* of field quantisation — in particular the parallels to the quantisation scheme employed in the previous example. For the *evaluation* of the resulting quantised theory we refer the reader to the literature. An excellent exposition of QED and its applications can be found, e.g., in Ryder's book [19].

The starting point of the quantisation scheme is again a classical variational principle. In other words we start out from a formulation where the *classical* physics of electromagnetic fields is derived from a Lagrangian function. As shown within the framework of classical relativistic electrodynamics (cf., e.g., Jackson's book) the source-free Maxwell equations can be generated from the action

$$\boxed{S[A] = \int d^4x \mathcal{L}(A), \qquad \mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu},}$$

where $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ is the electromagnetic field tensor, and $A = (\phi, \mathbf{A})^T$ is the 4-vector potential ($c = 1$). The Lagrangian above has the property of being (a) gauge invariant, and (b) exhibiting the solutions of the free Maxwell equations

$$\boxed{\partial_\mu F^{\mu\nu} = 0}$$

as its extremal field configurations.[11]

[11] To see this, one applies the usual variational principle,

$$\frac{\delta S[A]}{\delta A(x)} = 0.$$

To work with the Lagrangian density $\mathcal{L}$ one needs to specify a gauge. (As a parenthetical remark we mention that the necessity to gauge fix is in fact a source of notorious difficulties in gauge field theories in general. However, these problems are of little concern for the present discussion.) Here we chose the so-called radiation or Coulomb gauge $\phi = 0$, $\nabla \cdot \mathbf{A} = 0$, thereby reducing the number of independent components of A from four to two. The next step towards a quantised theory is again to introduce canonical momenta. In analogy to section 1.1.2 we define $\pi^\mu = \partial_{\dot{A}_\mu}\mathcal{L}$ which leads to

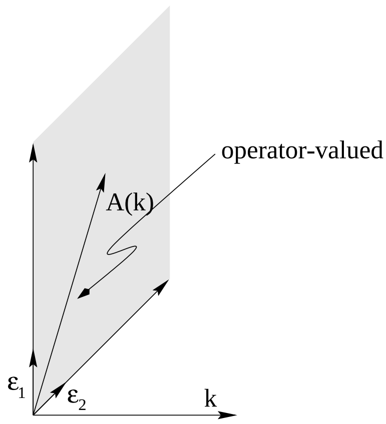
$$\pi^0 = \partial_{\dot{A}_0}\mathcal{L} = 0, \qquad \pi^i = \partial_{\dot{A}_i}\mathcal{L} = \partial^0 A^i - \partial^i A^0 = E^i,$$

where $\mathbf{E}$ is the electric field.[12]

Quantising the field theory now again amounts to introducing operators $A_i \mapsto \hat{A}_i$, $\pi_i \mapsto \hat{\pi}_i$, as well as canonical commutation relations between $\hat{A}_i$ and $\hat{\pi}_j$. A natural *Ansatz* for the commutation relations would be

$$[\hat{A}_i(\mathbf{x}, t), \hat{\pi}^j(\mathbf{x}', t)] = -[\hat{A}^i(\mathbf{x}, t), \hat{\pi}^j(\mathbf{x}', t)] = i\delta_{ij}\delta(\mathbf{x} - \mathbf{x}'). \tag{1.20}$$

Yet a closer inspection reveals that these identities are in fact in conflict with the Coulomb gauge $\nabla \cdot \mathbf{A} = 0$ (cf. Ref. [19], pp. 142). The way out is to replace δ_{ij} by a more general symmetric tensor. However as this complication does not alter the general *principle* of quantisation we do not discuss them any further here. The further construction of the theory is conceptually analogous to the phonon model and will be sketched only briefly.



Again one introduces momentum 'modes' by Fourier transforming the field:

$$\hat{A}_i(x) = \int \frac{d^3k}{(2\pi)^3 2k_0} \sum_{\lambda=1,2} \epsilon^{(\lambda)}(k) \left[a^{(\lambda)}(k)e^{-ikx} + \hat{a}^{(\lambda)\dagger}(k)e^{ikx}\right], \tag{1.21}$$

where $k^2 \equiv k_0^2 - \mathbf{k}^2 = 0$,[13] $\epsilon^{(\lambda)}(k)$ are polarisation vectors (cf. Fig. 1.2) obeying $\mathbf{k} \cdot \epsilon^{(\lambda)}(k) = 0$ (Coulomb gauge!). The specific form of the integration measure follows from the general

[12] The definitions above differ from the analogous equation (1.11) in so far as (a) the fields carry an additional discrete index $i = 1, \dots 4$ — they are 'vector' rather than 'scalar' fields — and (b) that the indices appear as upper and sometimes as lower indices, where upper and lower indices are connected with each other by an application of the Minkowskii metric tensor. Both aspects are of little significance for the present discussion.

[13] The condition $k \cdot k = 0$ follows from the Coulomb gauge formulation of Maxwell's equations, $\partial_\mu \partial^\mu A_\nu = 0$.

condition of relativistic invariance (cf. Ref. [19], pp. 143). Substituting this representation into the Hamilton operator of the field theory one obtains

$$\hat{H} = \sum_\lambda \int \frac{d^3k}{(2\pi)^3 2k_0} \frac{k_0}{2} a^{(\lambda)\dagger}(k) a^{(\lambda)}(k). \tag{1.22}$$

As Eq. (**??**), this is an oscillator type Hamiltonian. The difference is that the operators a generate oscillator quanta of the quantised electromagnetic field, so-called transverse **photons**, rather than phonons. Eq. (1.21) represents the decomposition of the free quantised vector potential in terms of photons. As with phonons, the oscillator quanta of the electromagnetic field can also be interpreted as particles. In this sense, the decomposition (1.21) represents the bridge between the wave and the particle description of electrodynamics. For discussions of the physical applications of the theory — in both high energy and condensed matter physics — we refer the reader to the literature, e.g. Ref. [19] (high energy) and Ref. [1] (condensed matter).