Chapter 11

Field theory: from phonons to photons

In our survey of single- and "few"-particle quantum mechanics, it has been possible to work with a discrete representation in which we index individual constituent particles. However, when the "elementary excitations" of the system involve the coherent *collective* motion of many individual discrete particle degrees of freedom – such as the wave-like atomic vibrations of an ordered elastic solid, or where discrete underlying classical particles can not even be identified – such as the electromagnetic field, such a representation is inconvenient or even inaccessible. In such cases, it is useful to turn to a continuum formulation of quantum mechanics. In the following, we will develop these fundamental ideas on the background of the simplest continuum theory: lattice vibrations of the atomic chain. As we will see, this study will provide a platform to investigate the quantum mechanics of the electromagnetic field – the subject of quantum electrodynamics – and will pave the way to the development of quantum field theory of relativistic particles.

11.1 Quantization of the classical atomic chain

As a simplified model of an ordered (one-dimensional) crystal, let us consider a chain of point particles each of mass m (atoms) which are elastically connected by springs with spring constant k_s (chemical bonds) (see Fig. 11.1). Although our target will be to construct a *quantum* theory of the elementary vibrational excitations, it is helpful to begin our analysis by reviewing the classical properties of the system.

11.1.1 Classical chain

For reasons that will become clear, it is instructive to consider the **Lagrangian formulation** of the problem. For the N-atom chain, the classical Lagrangian is given by,

$$L = T - V = \sum_{n=1}^{N} \left[\frac{m}{2} \dot{x}_n^2 - \frac{k_s}{2} (x_{n+1} - x_n - a)^2 \right], \tag{11.1}$$

where the first term accounts for the kinetic energy of the particles whilst the second describes their coupling.[1] For convenience, we adopt periodic boundary

[1] In real solids, the inter-atomic potential is, of course, more complex than our quadratic approximation. Yet, for "weak coupling", the harmonic contribution dominantes (cf. our discussion of molecular vibrations). For the sake of simplicity we, therefore, neglect the effects caused by higher order contributions.

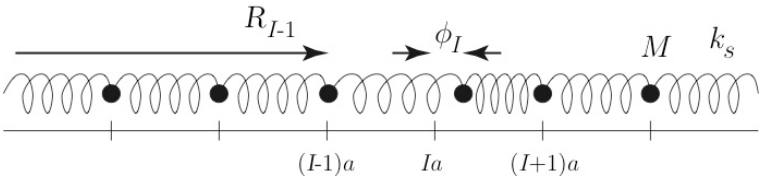


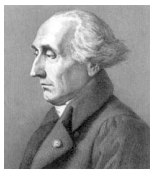
Figure 11.1: Toy model of a one-dimensional solid: a chain of point-like particles each of mass m coupled elastically by springs with spring constant k_s.

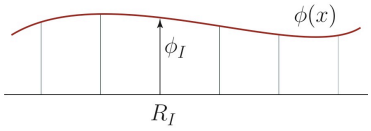
conditions such that $x_{N+1} \equiv Na + x_1$ where a denotes the "natural" equilibrium lattice spacing. Anticipating that the effect of lattice vibrations on the solid is weak (i.e. long-range atomic order is maintained) we will assume that (a) the n-th atom has its equilibrium position at $\bar{x}_n \equiv na$, and (b) that the deviation from the equilibrium position remains 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 (11.1) then takes the form

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

Now, typically, we are not concerned with the behaviour of a given system on 'atomic' length scales. (For such purposes, our model is in any case much to primitive!) Rather, we are interested in **universal** features, i.e. experimentally observable behaviour, common to a wide range of physical systems, that manifests itself on macroscopic length scales where the detailed form of the model is inessential. For example, we 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 **continuum approximation**, 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. In the present case, taking a continuum limit amounts to describing the lattice displacements ϕ_n in terms of *smooth functions*, $\phi(x)$ of a continuous variable x (see figure). Clearly such a description makes sense only if relative fluctuations on atomic scales are weak (for otherwise the smoothness condition would be violated).

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 of 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.





▷ EXERCISE. Starting with the discrete form of the Lagrangian, or otherwise, show the classical equations of motion take the form,

$$m\ddot{\phi}_n = k_s a^2 (\phi_{n+1} - 2\phi_n + \phi_{n-1}).$$

Remembering that the boundary conditions are periodic, obtain the normal modes. From this result, determine the condition under which the continuum approximation can be justified.

Hint: consider the ansatz, $\phi_n(t) = e^{i(kna - \omega t)}$.

Introducing continuum degrees of freedom, $\phi(x)$, and applying a first order Taylor expansion,[2] we can define

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

[2]Indeed, for reasons that will become clear, higher order contributions to the Taylor expansion do not contribute to the low-energy properties of the system where the continuum approximation is valid.

where $L = Na$ (not to be confused with the Lagrangian itself!) denotes the total length of the chain. Expressed in terms of the new degrees of freedom, the continuum limit of the Lagrangian then reads $L[\phi] = \int_0^L dx\, \mathcal{L}(\dot{\phi}, \phi)$, where

$$\boxed{\mathcal{L}(\dot{\phi}, \phi) = \frac{\rho}{2}\dot{\phi}^2 - \frac{\kappa_s a^2}{2}(\partial_x \phi)^2\,,} \tag{11.2}$$

denotes the Lagrangian density, $\rho = m/a$ denotes the mass per unit length and $\kappa_s = k_s/a$. The corresponding **classical action** is given by

$$\boxed{S[\phi] = \int dt\, L[\phi]\,.} \tag{11.3}$$

Thus, we have succeeded in trading the N-point particle description in for one involving *continuous* degrees of freedom, $\phi(x)$, a **(classical) field**. The dynamics of the latter are specified by "functionals" $L[\phi]$ and $S[\phi]$ which represent the continuum generalizations of the discrete classical Lagrangian and action, respectively.[3] However, although we have achieved a continuum formulation, we have yet to extract concrete physical information from the action. To do so, we need to derive equations of motion. At first sight, it may not be entirely clear what is meant by 'equations of motion' in the context of an infinite dimensional model. The answer to this question lies in Hamilton's extremal principle of classical mechanics:

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.

▷ INFO. **Hamilton's extremal principle:** 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 realized are those that extremize the action. This means that, for any smooth curve $y(t)$,

$$\lim_{\epsilon \to 0} \frac{1}{\epsilon}(S[x + \epsilon y] - S[x]) = 0\,, \tag{11.4}$$

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 $x(t)$ obeys the **Euler-Lagrange equation** of motion (exercise),

$$\boxed{\frac{d}{dt}(\partial_{\dot{x}} L) - \partial_x L = 0\,.} \tag{11.5}$$

Now, in Eq. (11.3), 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 (11.3) is subjected to an extremal principle analogous to Eq. (11.4). To do so, we must effect the substitution $\phi(x, t) \to \phi(x, t) + \epsilon\eta(x, t)$ into Eq. (11.3) and demand that the contribution first order in ϵ vanishes. When applied to the specific Lagrangian (11.2), a substitution of the of the 'varied' field leads to

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

Integrating by parts (with respect to time for the first term under the integral, and space in the second) and demanding that the contribution linear

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

in ϵ vanishes, one obtains $\int dt \int_0^L dx(\rho\ddot{\phi} - \kappa_s a^2 \partial_x^2 \phi)\eta = 0$. (Notice that the boundary terms associated with both t and x vanish identically.[4] Now, since η was defined to be any 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**,

$$\boxed{\rho\ddot{\phi} = \kappa_s a^2 \partial_x^2 \phi\,.} \tag{11.6}$$

The solutions of Eq. (11.6) have the general form $\phi_+(x+vt) + \phi_-(x-vt)$ where $v = a\sqrt{\kappa_s/\rho}$, and $\phi_\pm$ are arbitrary smooth functions of their 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 figure). 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. With this background, let us now turn to the consider the quantization of the quantum mechanical chain.

11.1.2 Quantum chain

In addressing the quantum description, the first question to ask is a conceptual one: is there a general methodology to quantize models of the form described by the atomic chain (11.2)? Indeed, there is a standard procedure to quantize continuum theories which closely resembles the quantization 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 generalization of the definition $p_n \equiv \partial_{\dot{x}_n} L$ of point mechanics to a continuum suggests setting

$$\boxed{\pi = \partial_{\dot{\phi}} \mathcal{L}(\dot{\phi}, \phi)\,.} \tag{11.7}$$

In common with $\phi(x,t)$, the **canonical momentum**, $\pi(x,t)$, is a continuum degree of freedom. At each space point it may take an independent value. From the Lagrangian, we can define the Hamiltonian, $H[\phi,\pi] \equiv \int dx\, \mathcal{H}(\phi,\pi)$, where $\mathcal{H}(\phi,\pi) \equiv \pi\dot{\phi} - \mathcal{L}(\dot{\phi},\phi)$. represents the **Hamiltonian density**. Applied to the atomic chain (11.2), the canonical momentum $\pi = \rho\dot{\phi}$ and $\mathcal{H}(\phi,\pi) = \frac{\pi^2}{2\rho} + \frac{\kappa_s a^2}{2}(\partial_x\phi)^2$.

In this form, the Hamiltonian can be quantized according to the following rules: (a) promote the fields $\phi(x)$ and $\pi(x)$ to operators: $\phi \mapsto \hat{\phi}$, $\pi \mapsto \hat{\pi}$, and (b) generalise the canonical commutation relations of one-particle quantum mechanics, $[\hat{p}_m, x_n] = -i\hbar\delta_{mn}$, according to the relation[5]

$$\boxed{[\hat{\pi}(x), \hat{\phi}(x')] = -i\hbar\delta(x-x')\,.} \tag{11.8}$$

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

$$\boxed{\hat{\mathcal{H}}(\hat{\phi},\hat{\pi}) = \frac{1}{2\rho}\hat{\pi}^2 + \frac{\kappa_s a^2}{2}(\partial_x\hat{\phi})^2\,.}$$

[4] If we assume that the function ϕ already obeys the boundary conditions, we must have $\eta(0,t) = \eta(L,t) = \eta(x,0) = \eta(x,T) = 0$).

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

▷ EXERCISE. To develop this field theoretical formulation of the Hamiltonian, we have pursued a Lagrangian formulation. If you feel uncertain about this methodology, you should explore the derivation of $\hat{H}$ directly from the discrete atomic formulation. First, show that, for the discrete harmonic chain, the classical Hamiltonian is given by

$$\hat{H} = \sum_n \left[\frac{p_n^2}{2m} + \frac{k_s}{2}(\phi_{n+1} - \phi_n)^2 \right] .$$

Promoting the displacements and momenta to operators, and applying the canonical quanitization conditions, $[\hat{p}_n, \phi_{n'}] = -i\hbar\delta_{nn'}$, obtain the discrete form of the Hamiltonian. Taking the continuum limit, show that the Hamiltonian recovers the continuum form derived through the Lagrangian formulation.

The Hamiltonian represents a quantum field theoretical *formulation* of the problem but not yet a *solution*. To address the quantum properties of the system, it is helpful now to switch to a Fourier representation. As with any function, operator-valued functions can be represented in a variety of different ways. In particular they can be subjected to Fourier expansion,

$$\left\{ \begin{matrix} \hat{\phi}_k \\ \hat{\pi}_k \end{matrix} \right. \equiv \frac{1}{L^{1/2}} \int_0^L dx \; e^{\{\mp ikx} \left\{ \begin{matrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{matrix} \right. , \qquad \left\{ \begin{matrix} \hat{\phi}(x) \\ \hat{\pi}(x) \end{matrix} \right. = \frac{1}{L^{1/2}} \sum_k e^{\{\pm ikx} \left\{ \begin{matrix} \hat{\phi}_k \\ \hat{\pi}_k \end{matrix} \right. , \tag{11.9}$$

where $\sum_k$ represents the sum over all Fourier coefficients indexed by quantized wavevectors $k = 2\pi m/L$, m integer. Note that, since the classical field $\phi(x)$ is *real*, the quantum field $\hat{\phi}(x)$ is *Hermitian*, i.e. $\hat{\phi}_k = \hat{\phi}_{-k}^\dagger$ (and similarly for $\hat{\pi}_k$). In the Fourier representation, the transformed field operators obey the canonical commutation relations (exercise),

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

▷ EXERCISE. Making use of Eqs. (11.8) and (11.9) derive the canonical commutation relation above.

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

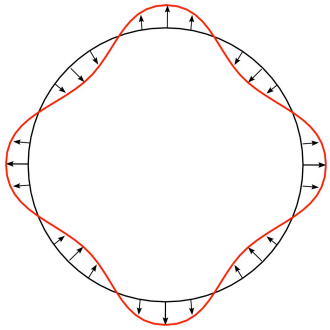
$$\int_0^L dx \, (\partial\hat{\phi})^2 = \sum_{k,k'} (ik\hat{\phi}_k)(ik'\hat{\phi}_{k'}) \overbrace{\frac{1}{L}\int_0^L dx \, e^{i(k+k')x}}^{\delta_{k+k',0}} = \sum_k k^2 \hat{\phi}_k \hat{\phi}_{-k} ,$$

together with the parallel relation for $\int_0^L dx \, \hat{\pi}^2$, the Hamiltonian assumes the "near diagonal" form,

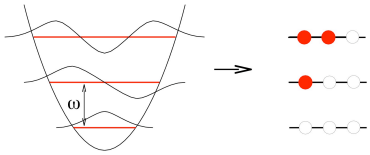
$$\hat{H} = \sum_k \left[\frac{1}{2\rho}\hat{\pi}_k\hat{\pi}_{-k} + \frac{1}{2}\rho\omega_k^2 \, \hat{\phi}_k\hat{\phi}_{-k} \right] , \tag{11.10}$$

where $\omega_k = v|k|$, and $v = a(\kappa_s/\rho)^{1/2}$ denotes the classical sound wave velocity. In this form, the Hamiltonian can be identified as nothing more than a superposition of independent quantum harmonic oscillators. The only difference between (11.10) and the canonical form of an oscillator Hamiltonian $H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2$ is the presence of sub-indices k and $-k$ (a consequence of $\hat{\phi}_k^\dagger = \hat{\phi}_{-k}$). As we will show shortly, this difference is inessential. This

result is actually not difficult to understand (see figure): Classically, the system supports a discrete set of wave-like excitations, each indexed by a wave number $k = 2\pi m/L$. Within the quantum picture, each of these excitations is described by an oscillator Hamiltonian 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.) To understand how this programme can be achieved let us recall the properties of the quantum harmonic oscillator.



▷ INFO. In quantum mechanics, the **harmonic oscillator** has the status of a single-particle problem. However, the fact that the energy levels, $\epsilon_n = \hbar\omega(n + 1/2)$, 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 figure.) 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 $a \equiv \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} + \frac{i}{m\omega}\hat{p})$, $a^\dagger \equiv \sqrt{\frac{m\omega}{2\hbar}}(\hat{x} - \frac{i}{m\omega}\hat{p})$. Up to a factor of i, the transformation $(\hat{x}, \hat{p}) \to (a, a^\dagger)$ is canonical, i.e. the new operators obey the canonical commutation relation, $[a, a^\dagger] = 1$. More importantly, in the a-representation, the Hamiltonian takes the simple form, $\hat{H} = \hbar\omega(a^\dagger a + 1/2)$, as can be checked by direct substitution. The complete hierarchy of higher energy states can be generated by setting $|n\rangle \equiv \frac{1}{\sqrt{n!}}(a^\dagger)^n|0\rangle$.

While the a-representation provides another way of constructing eigenstates of the quantum harmonic oscillator, its real advantage is that it naturally affords a many-particle interpretation. Temporarily forgetting about the original definition of the oscillator, we can *declare* $|0\rangle$ to be a 'vacuum' state, i.e. a state with no particles present. $a^\dagger|0\rangle$ then represents a state with a single featureless particle (the operator $a^\dagger$ does not carry any quantum number labels) of energy $\hbar\omega$. Similarly, $(a^\dagger)^n|0\rangle$ is considered as a many-body state with n particles, i.e. within the new picture, $a^\dagger$ 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 $a^\dagger a|n\rangle = n|n\rangle$, 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 fulfils our objective: it allows an interpretation of the excited states of the harmonic oscillator as a superposition of independent structureless entities.

With this background, we may return to the harmonic atomic chain (11.10)

and, inspired by the ladder operator formalism, define[6]

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

With this definition, one finds that the ladder operators obey the commutation relations (exercise)

$$[a_k, a_{k'}^\dagger] = \delta_{kk'}, \qquad [a_k, a_{k'}] = [a_k^\dagger, a_{k'}^\dagger] = 0\,, \tag{11.11}$$

and the Hamiltonian assumes the diagonal form

$$\boxed{\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2}\right).} \tag{11.12}$$

Eqs. (11.11) and (11.12) represent the final result of our analysis: The low-lying elementary excitations of the discrete atomic chain are described by oscillator wave-like modes – known as **phonons** – each characterised by a wavevector k and a linear dispersion, $\omega_k = v|k|$. A generic state of the system is given by

$$|\{n_k\} = (n_1, n_2, \cdots)\rangle = \frac{1}{\sqrt{\prod_i n_i!}}(a_{k_1}^\dagger)^{n_1}(a_{k_2}^\dagger)^{n_2}\cdots|0\rangle\,.$$

The representation derived above illustrates the capacity to think about quantum problems in different complementary "pictures", a principle that finds innumerable applications. 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, the 'fictitious' quasi-particle states of the harmonic chain, the phonons, *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 'real' particles.

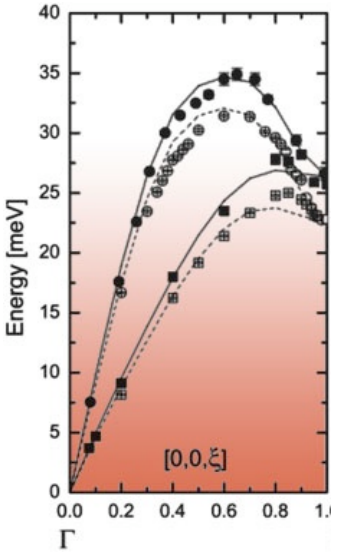


Figure shows a typical measured phonon dispersion of an ordered crystalline solid obtained by neutron scattering. The x-axis indexes wavenumbers along a lattice direction (specified in units of π/a). Three generic aspects are visible: (1) near $k = 0$, the dispersion is, as expected, linear. (2) The several branches are associated with different "polarizations" of the lattice fluctuations. (3) For wavelengths comparable to the lattice spacing, $k \sim \pi/a$, non-universal features specific to the particular material become visible.

▷ EXAMPLE: **Debye theory of solids:** Our analysis above focussed on the longitudinal vibrations of the one-dimensional atomic chain. In three-dimensions, each mode is associated with three possible polarizations, λ: two transverse and one longitudinal. Taking into account all degrees of freedom, it is straightforward to show that the generalized Hamiltonian takes the form,

$$\hat{H} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left(a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k},\lambda} + \frac{1}{2}\right),$$

where, for simplicity, we assume that the dispersion, $\omega_{\mathbf{k}} = v|\mathbf{k}|$ is independent of polarization. Let us use this result to obtain the internal energy and specific heat due to phonons. Now, for an equilibrium thermal distribution, the average phonon occupancy of state $(\mathbf{k}, \lambda)$ is given simply by the Bose-Einstein distribution, $n_{\rm B}(\hbar\omega_{\mathbf{k}}) \equiv \frac{1}{e^{\hbar\omega_{\mathbf{k}}/k_{\rm B}T}-1}$. The internal energy is therefore given by

$$E = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}}(n_{\rm B}(\hbar\omega_{\mathbf{k}}) + 1/2) = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}}\left[\frac{1}{e^{\hbar\omega_{\mathbf{k}}/k_{\rm B}T}-1} + \frac{1}{2}\right].$$

In the thermodynamic limit, where $N \equiv V/a^3 \to \infty$, we may replace the sum over modes by an integral, $\sum_{\mathbf{k}} \to V\int_0^{k_{\rm D}} \frac{d^3k}{(2\pi)^3} = \frac{V}{2\pi^2}\int_0^{k_{\rm D}} k^2\,dk$, where $k_{\rm D}$, denotes the

Peter Josephus Wilhelmus Debye 1884-1966: Dutch-American physicist renowned for his work on molecular structure, especially dipole moments and the diffraction of X-rays and electrons in gases. Debye was awarded a Nobel Prize in Chemistry, 1936, "for his contributions to our knowledge of molecular structure through his investigations on dipole moments and on the diffraction of X-rays and electrons in gases".

[6] 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 conjuate.

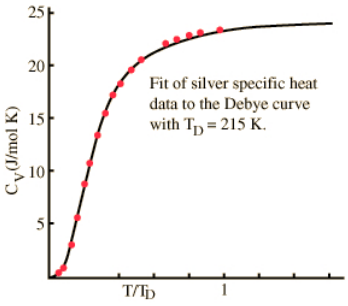
largest wave vector accessible in the crystal. We can fix $k_{\rm D}$ by ensuring that the total number of modes (for each polarization) matches the total number of degrees of freedom, i.e. $\frac{1}{(2\pi)^3/V}\frac{4}{3}\pi k_{\rm D}^3 = N$, i.e. $k_{\rm D} = \frac{(6\pi^2)^{1/3}}{a}$. The corresponding frequency scale, $\omega_{\rm D} = vk_{\rm D}$, is known as the **Debye frequency**. In this limit, dropping the temperature independent contribution from zero point fluctuations, the internal energy per particle is given by

$$\varepsilon \equiv \frac{E}{N} = \frac{3a^3}{2\pi^2}\int_0^{k_{\rm D}} k^2\, dk\, \frac{\hbar v k}{e^{\hbar v k/k_{\rm B}T}-1}\,.$$

Then, defining the **Debye temperature**, $T_{\rm D} = \hbar v k_{\rm D}/k_{\rm B}$, we have $\varepsilon = 9k_{\rm B}T(\frac{T}{T_{\rm D}})^3\int_0^{T_{\rm D}/T}$ The corresponding specific heat per particle can be obtained from the temperature derivative and leads to

$$c_V = 9k_{\rm B}\left(\frac{T}{T_{\rm D}}\right)^3\int_0^{T_{\rm D}/T}\frac{z^4\,dz}{(e^z-1)^2}\,.$$

In particular, at high temperatures, we recover the **Dulong-Petit law**, $c_V = 3k_{\rm B}$ following from the equipartition theorem – each degree of freedom is associated with an energy $k_{\rm B}T/2$. At low temperatures, $T \ll T_{\rm D}$, we may replace the upper limit on the integral by ∞ from which we find that $c_V \sim T^3$. Both limits compare well with experiment (see figure).



This completes our discussion of the classical and quantum field theory of the harmonic atomic chain. In this example, we have seen how we can effect a quantum formulation of a continuum system. Using the insights obtained in this example, we now turn to consider the quantization of the electromagnetic field.

11.2 Quantum electrodynamics

In common with the continuous formulation of the atomic chain, in vacua, the electromagnetic (EM) field satisfies a wave equation. The generality of the procedure outlined above suggests that the quantization of the EM field might therefore proceed in an entirely analogous manner. However, there are a number of practical differences that make quantization a slightly more difficult enterprise: Firstly, the vector character of the vector potential $\mathbf{A}$, alongside relativistic covariance, gives the problem a non-trivial internal geometry. Moreover, the gauge freedom of the vector potential introduces redundant degrees of freedom whose removal on the quantum level is not straightforward. To circumvent a lengthy discussion of these issues, we will not address the problem of EM field quantization in all its detail.[7] On the other hand, the photon field plays a much too important role in all branches of physics for us to drop the problem altogether. We will therefore aim at an intermediate exposition, largely insensitive to the problems outlined above but sufficiently general to illustrate the main principles. As with the harmonic chain, to prepare the way, we begin by developing the classical field theory of the EM field.

11.2.1 Classical theory of the electromagnetic field

In vacuum, the Lagrangian density of the EM field is given by $\mathcal{L} = -\frac{1}{4\mu_0}F_{\mu\nu}F^{\mu\nu}$ (summation convention implied) where $\mu_0 = 4\pi\times 10^{-7}\,{\rm Hm}^{-1}$ denotes the **vac-**

[7] Readers interested in a more thorough and illuminating exposition are referred to the literature, e.g., L. H. Ryder, *Quantum Field Theory* (Cambridge University Press, 1996), or the excellent lecture notes of Eduardo Fradkin that have been made available online at `http://webusers.physics.illinois.edu/ efradkin/phys582/physics582.html`.

uum permeability,

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu = \begin{pmatrix} 0 & -E_x/c & -E_y/c & -E_z/c \\ E_x/c & 0 & B_z & -B_y \\ E_y/c & -B_z & 0 & B_x \\ E_z/c & B_y & -B_x & 0 \end{pmatrix}_{\mu\nu}$$

denotes the EM field tensor, $\mathbf{E} = \dot{\mathbf{A}}$ is the electric field, and $\mathbf{B} = \nabla \times \mathbf{A}$ is the magnetic field. As a first step towards quantization, we must specify a gauge. In the absence of charge, a particularly convenient choice is the **Coulomb gauge**, $\nabla \cdot \mathbf{A} = 0$, with the scalar component $\phi = 0$.[8] Using these gauge conditions, one may verify that the classical Lagrangian assumes the form,

$$\boxed{L[\mathbf{A}(\mathbf{x},t)] = \frac{1}{2\mu_0}\int d^3x \left[\frac{1}{c^2}\dot{\mathbf{A}}^2 - (\nabla \times \mathbf{A})^2\right].} \tag{11.13}$$

The corresponding classical Euler-Lagrange equations of motion, $\partial_\mu F^{\mu\nu} = 0$, translate to the wave equation (exercise)

$$\boxed{\frac{1}{c^2}\ddot{\mathbf{A}} = \nabla^2 \mathbf{A}\,.}$$

The structural similarity between the EM field and the continuous formulation of the harmonic chain is clear. By analogy with our discussion above, we should now switch to the Fourier representation and quantize the classical field. However, in contrast to our analysis of the chain, we are now dealing (i) with the full three-dimensional Laplacian acting upon (ii) the vector field $\mathbf{A}$ that is (iii) subject to the constraint $\nabla \cdot \mathbf{A} = 0$. It is these aspects which lead to the complications outlined above.

We can circumvent these difficulties by considering cases where the geometry of the system reduces the complexity of the eigenvalue problem while still retaining the key conceptual aspects of the problem. This restriction is less artificial than it might appear. For example, just as the field ϕ in the classical atomic chain can be expanded in Fourier harmonics, in long waveguides, the EM vector potential can be expanded in solutions of the eigenvalue equation[9]

$$-\nabla^2 \mathbf{u}_k(\mathbf{x}) = \lambda_k \mathbf{u}_k(\mathbf{x}), \tag{11.14}$$

where k denotes a discrete *one-dimensional* index, and the vector-valued functions $\mathbf{u}_k$ are real and orthonormalized, $\int d^3x\, \mathbf{u}_k \cdot \mathbf{u}_{k'} = \delta_{kk'}$. The dependence of the eigenvalues λ_k on k depends on details of the geometry and need not be specified for the moment.

▷ INFO. An **electrodynamic waveguide** is a quasi one-dimensional cavity with metallic boundaries (see Fig. 11.2). The practical advantage of waveguides is that they are good at confining EM waves. At large frequencies, where the wavelengths are of order meters or less, radiation loss in conventional conductors is high. In these frequency domains, hollow conductors provide the only practical way of transmitting radiation. EM field propagation inside a waveguide is constrained by boundary conditions. Assuming the walls of the system to be perfectly conducting,

$$\mathbf{E}_\parallel(\mathbf{x}_\mathrm{b}) = 0, \qquad \mathbf{B}_\perp(\mathbf{x}_\mathrm{b}) = 0\,, \tag{11.15}$$

[8] Keep in mind that, once a gauge has been set, we cannot expect further results to display "gauge invariance."

[9] More precisely, one should say that Eq. (11.14) defines the set of eigenfunctions relevant for the *low-energy* dynamics of the waveguide. More complex eigenfunctions of the Laplace operator exist but they involve much higher energy.

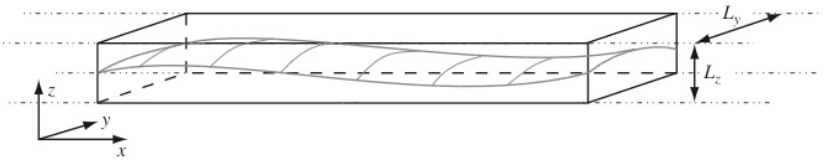


Figure 11.2: EM waveguide with rectangular cross-section. The structure of the eigenmodes of the EM field is determined by boundary conditions at the walls of the cavity.

where $\mathbf{x}_\mathrm{b}$ parameterize points on the boundary of the system, and $\mathbf{E}_\parallel$ ($\mathbf{B}_\perp$) is the parallel (perpendicular) component of the electric (magnetic) field. Applied to the problem at hand, let us consider a long cavity with uniform rectangular cross-section $L_y \times L_z$. To conveniently represent the Lagrangian of the system, we wish to express the vector potential in terms of eigenfunctions $\mathbf{u_k}$ that are consistent with the boundary conditions (11.15). A complete set of functions fulfilling this condition is given by

$$\mathbf{u_k} = \mathcal{N}_k \begin{pmatrix} c_1 \cos(k_x x)\sin(k_y y)\sin(k_z z) \\ c_2 \sin(k_x x)\cos(k_y y)\sin(k_z z) \\ c_3 \sin(k_x x)\sin(k_y y)\cos(k_z z) \end{pmatrix} .$$

Here $k_i = n_i\pi/L_i$, with $i = x, y, z$ and n_i is integer, $\mathcal{N}_k$ is a factor normalizing $\mathbf{u_k}$ to unit modulus, and the coefficients c_i are subject to the condition $c_1k_x + c_2k_y + c_3k_z = 0$ (reflecting the gauge choice $\nabla \cdot \mathbf{A} = 0$). Indeed, it is straightforward to verify that a general superposition of the type $\mathbf{A}(\mathbf{x}, t) \equiv \sum_\mathbf{k} \alpha_\mathbf{k}(t)\mathbf{u_k}(\mathbf{x})$, $\alpha_\mathbf{k}(t) \in \mathbb{R}$, is divergenceless, and generates an EM field compatible with (11.15). Substitution of $\mathbf{u_k}$ into (11.14) identifies the eigenvalues as $\lambda_\mathbf{k} = k_x^2 + k_y^2 + k_z^2$.

In the physics and electronic engineering literature, eigenfunctions of the Laplace operator in a quasi-one-dimensional geometry are commonly described as **modes**. As we will see shortly, the energy of a mode (i.e. the Hamiltonian evaluated on a specific mode configuration) grows with $\lambda_\mathbf{k}$. In cases where one is interested in the low-energy dynamics of the EM field, only configurations with small $\lambda_\mathbf{k}$ are relevant. For example, let us consider a massively anisotropic waveguide with $L_z < L_y \ll L_x$. In this case the modes with smallest λ_k are those with $k_z = 0$, $k_y = \pi/L_y$, and $k_x \equiv k \ll L_{z,y}^{-1}$. With this choice,

$$\mathbf{u}_k = \frac{2}{\sqrt{V}} \sin(\pi y/L_y)\sin(kx)\,\hat{\mathbf{e}}_z, \qquad \lambda_k = k^2 + \left(\frac{\pi}{L_y}\right)^2 , \tag{11.16}$$

and a scalar index k suffices to label both eigenvalues and eigenfunctions $\mathbf{u}_k$. A caricature of the spatial structure of the functions $\mathbf{u}_k$ is shown in Fig. 11.2.

Returning to the problem posed by (11.13) and (11.14), one can expand the vector potential in terms of eigenfunctions $\mathbf{u}_k$ as $\mathbf{A}(\mathbf{x}, t) = \sum_k \alpha_k(t)\mathbf{u}_k(\mathbf{x})$, where the sum runs over all allowed values of the index parameter k. (In a waveguide of length L, $k = \pi n/L$ with n integer.) Substituting this expansion into (11.13), and using the normalization properties of $\mathbf{u}_k$, we obtain the Lagrangian,

$$L[\dot\alpha, \alpha] = \frac{1}{2\mu_0} \sum_k \left[\frac{1}{c^2}\dot\alpha_k^2 - \lambda_k \alpha_k^2\right] ,$$

i.e. a decoupled representation where the system is described in terms of independent dynamical systems with coordinates α_k. From this point on, the quantization procedure mirrors that of the atomic chain.

11.2.2 Quantum field theory of the electromagnetic field

To achieve the electromagnetic field quantization, we first define the canonical momenta through the relation,

$$\pi_k = \partial_{\dot{\alpha}_k} \mathcal{L} = \epsilon_0 \dot{\alpha}_k \,,$$

where $\epsilon_0 = 1/\mu_0 c^2$ denotes the **vacuum permittivity**, which leads to the classical Hamiltonian $H = \sum_k (\frac{1}{2\epsilon_0}\pi_k^2 + \frac{1}{2}\epsilon_0 c^2 \lambda_k \alpha_k^2)$. Next we quantize the theory by promoting fields to operators $\alpha_k \to \hat{\alpha}_k$ and $\pi_k \to \hat{\pi}_k$, and declare the canonical commutation relations $[\hat{\pi}_k, \hat{\alpha}_{k'}] = -i\hbar\delta_{kk'}$. The quantum Hamiltonian operator, again of harmonic oscillator type, then reads

$$\hat{H} = \sum_k \left[\frac{\hat{\pi}_k^2}{2\epsilon_0} + \frac{1}{2}\epsilon_0 \omega_k^2 \hat{\alpha}_k^2 \right] ,$$

where $\omega_k^2 = c^2 \lambda_k$.

Then, guided by the analysis of the atomic chain, we now introduce the ladder operators,

$$a_k = \sqrt{\frac{\epsilon_0 \omega_k}{2\hbar}} \left(\hat{\alpha}_k + \frac{i}{\epsilon_0 \omega_k} \hat{\pi}_k \right) , \qquad a_k^\dagger = \sqrt{\frac{\epsilon_0 \omega_k}{2\hbar}} \left(\hat{\alpha}_k - \frac{i}{\epsilon_0 \omega_k} \hat{\pi}_k \right) ,$$

whereupon the Hamiltonian assumes the now familiar form

$$\boxed{\hat{H} = \sum_k \hbar\omega_k \left(a_k^\dagger a_k + \frac{1}{2} \right) .} \tag{11.17}$$

For the specific problem of the first excited mode in a waveguide of width L_y, $\hbar\omega_k = c[k^2 + (\pi/L_y)^2]^{1/2}$. Eq. (11.17) represents our final result for the quantum Hamiltonian of the EM waveguide. Before concluding this section let us make a few comments on the structure of the result.

- ▷ Firstly, notice that the construction above almost completely paralleled our previous discussion of the atomic chain.[10] The structural similarity between the two systems finds its origin in the fact that the free field Lagrangian (11.13) is quadratic in the fields and, therefore, bound to map onto an oscillator-type Hamiltonian. That we obtained a simple *one-dimensional* superposition of oscillators is due to the boundary conditions specific to a narrow waveguide. For less restrictive geometries, e.g. free space, a more complex superposition of vectorial degrees of freedom in three-dimensional space would have been obtained (see below). However, the principal mapping of the free EM field onto a superposition of oscillators is independent of geometry.

- ▷ Physically, the quantum excitations described by (11.17) are, of course, the **photons** of the EM field. The unfamiliar appearance of the dispersion ω_k is again a peculiarity of the waveguide. However, in the limit of large longitudinal wave numbers $k \gg L_y^{-1}$, the dispersion approaches $\omega_k \simeq c|k|$, i.e. the familiar linear (relativistic) dispersion of the photon field. Also notice that, due to the equality of the Hamiltonians (11.12) and (11.17), all that has been said about the behavior of the phonon modes of the atomic chain carries over to the photon modes of the waveguide.

[10] Technically, the only difference is that, instead of index pairs $(k, -k)$, all indices (k, k) are equal and positive. This can be traced back to the fact that we have expanded in terms of the real eigenfunctions of the closed waveguide instead of the complex eigenfunctions of the periodic oscillator chain.

▷ As with their phonon analogue, the oscillators described by (11.17) exhibit zero-point fluctuations. It is a fascinating aspect of quantum electrodynamics that these oscillations, caused by quantization of *the* most relativistic field, surface at various points of non-relativistic physics, e.g. the attraction of two conducting plates in vacuum – the **Casimir effect**.

With the analysis of the waveguide complete, let us go back and consider the quantitization of the full three-dimensional system. For the waveguide, we have found that the vector potential can be expanded in modes of the cavity as $\hat{\mathbf{A}}(\mathbf{x}) = \sum_k \hat{\alpha}_k \mathbf{u}_k$ where, rearranging the expressions for the ladder operators, $\hat{\alpha}_k = \sqrt{\frac{\hbar}{2\epsilon_0\omega_k}}(a_k + a_k^\dagger)$. More generally, in a fully three-dimensional cavity, one may show that[11]

$$\hat{\mathbf{A}}(\mathbf{x}) = \sum_{\mathbf{k}\lambda=1,2} \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}V}} \left[\hat{\mathbf{e}}_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} e^{i\mathbf{k}\cdot\mathbf{x}} + \hat{\mathbf{e}}^*_{\mathbf{k}\lambda} a^\dagger_{\mathbf{k}\lambda} e^{-i\mathbf{k}\cdot\mathbf{x}}\right] ,$$

where V denotes the volume of the system, $\omega_{\mathbf{k}} = c|\mathbf{k}|$, and the two sets of polarization vectors, $\hat{\mathbf{e}}_{\mathbf{k}\lambda}$, are in general complex and normalized to unity, $\hat{\mathbf{e}}^*_{\mathbf{k}\lambda} \cdot \hat{\mathbf{e}}_{\mathbf{k}\lambda} = 1$. To ensure that the vector potential satifies the Coulomb gauge condition, we require that $\hat{\mathbf{e}}_{\mathbf{k}\lambda} \cdot \mathbf{k} = \hat{\mathbf{e}}^*_{\mathbf{k}\lambda} \cdot \mathbf{k} = 0$, i.e. the two polarization vectors are orthogonal to the wave vector. Two real vectors, $\hat{\mathbf{e}}_{\mathbf{k}\lambda}$ correspond to two linear polarizations while, for circular polarization, the vectors are complex. It is also convenient to assume that the two polarization vectors are mutually orthogonal, $\hat{\mathbf{e}}_{\mathbf{k}\lambda} \cdot \hat{\mathbf{e}}_{\mathbf{k}\mu} = \delta_{\mu\nu}$. The corresponding operators obey the commutation relations,

$$\boxed{[a_{\mathbf{k}\lambda}, a^\dagger_{\mathbf{k}'\lambda'}] = \delta_{\mathbf{k},\mathbf{k}'}\delta_{\lambda\lambda'}, \qquad [a_{\mathbf{k}\lambda}, a_{\mathbf{k}'\lambda'}] = 0 = [a^\dagger_{\mathbf{k}\lambda}, a^\dagger_{\mathbf{k}'\lambda'}] .}$$

With these definitions, the Hamiltonian then takes the familiar form

$$\boxed{\hat{H} = \sum_{\mathbf{k}\lambda} \hbar\omega_{\mathbf{k}} \left[a^\dagger_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} + 1/2\right] ,} \tag{11.18}$$

while, defining the vacuum, $|\Omega\rangle$, the eigenstates involve photon number states,

$$\boxed{|\{n_{\mathbf{k}\lambda}\}\rangle \equiv |\cdots, n_{\mathbf{k}\lambda}, \cdots\rangle = \prod_{\mathbf{k}\lambda} \frac{(a^\dagger_{\mathbf{k}\lambda})^{n_{\mathbf{k}\lambda}}}{\sqrt{n_{\mathbf{k}\lambda}!}} |\Omega\rangle .}$$

Finally, in practical applications (including our forthcoming study of radiative transitions in atoms), it is convenient to transfer the time-dependence to the operators by turning to the Heisenberg representation. In this representation, the field operators obey the Heisenberg equations of motion (exercise),

$$\dot{a}_{\mathbf{k}\lambda} = \frac{i}{\hbar}[\hat{H}, a_{\mathbf{k}\lambda}] = -i\omega_{\mathbf{k}} a_{\mathbf{k}\lambda} .$$

Integrating, we have $a_{\mathbf{k}\lambda}(t) = a_{\mathbf{k}\lambda}(0)e^{-i\omega_{\mathbf{k}}t}$, which translates to the relation

$$\boxed{\hat{\mathbf{A}}(\mathbf{x}, t) = \sum_{\mathbf{k}\lambda=1,2} \sqrt{\frac{\hbar}{2\epsilon_0\omega_{\mathbf{k}}V}} \left[\hat{\mathbf{e}}_{\mathbf{k}\lambda} a_{\mathbf{k}\lambda} e^{i(\mathbf{k}\cdot\mathbf{x}-\omega_{\mathbf{k}}t)} + \hat{\mathbf{e}}^*_{\mathbf{k}\lambda} a^\dagger_{\mathbf{k}\lambda} e^{-i(\mathbf{k}\cdot\mathbf{x}-\omega_{\mathbf{k}}t)}\right] .}$$

[11] In the infinite system, the mode sum becomes replaced by an integral, $\sum_{\mathbf{k}} \to \frac{V}{(2\pi)^3}\int d^3k$.