- The action of $\exp(\lambda N)$ on a coherent state, where λ is purely imaginary ($|\exp\lambda| = 1$), again gives a coherent state:

$$e^{\lambda N}|z\rangle = e^{\lambda N} e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}}|n\rangle = e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{z^n}{\sqrt{n!}} e^{\lambda n}|n\rangle$$
$$= e^{-|z|^2/2} \sum_{n=0}^{\infty} \frac{(e^{\lambda} z)^n}{\sqrt{n!}}|n\rangle = |e^{\lambda} z\rangle. \tag{11.35}$$

The relation $|\exp\lambda| = 1$ has been used only to obtain the last equality.
- The coherent states form an "overcomplete" basis:

$$\int \frac{\mathrm{dRe}\,z\,\mathrm{dIm}\,z}{\pi}\, |z\rangle\langle z| = I. \tag{11.36}$$

To prove this identity, we sandwich it between the bra $\langle n|$ and the ket $|m\rangle$. Setting $z = \rho\exp(i\theta)$, we have

$$\int \frac{\mathrm{dRe}\,z\,\mathrm{dIm}\,z}{\pi} \langle n|z\rangle\langle z|m\rangle = \int_0^{\infty} \rho\,\mathrm{d}\rho \int_0^{2\pi} \frac{\mathrm{d}\theta}{\pi} \frac{z^n z^{*m}}{\sqrt{n!m!}} e^{-\rho^2}$$
$$= \int_0^{\infty} \rho\,\mathrm{d}\rho \int_0^{2\pi} \frac{\mathrm{d}\theta}{\pi} \frac{\rho^{n+m}}{\sqrt{n!m!}} e^{i(n-m)\theta} e^{-\rho^2} = \delta_{nm},$$

where we have used the change of variable $\rho^2 = u$ and

$$\int_0^{\infty} \mathrm{d}u\, u^n e^{-u} = n!.$$

A direct consequence of (11.36) is that the "diagonal matrix elements" $\langle z|A|z\rangle$ are sufficient to completely define an operator A (Exercise 11.5.3).

These properties allow us easily to calculate the expectation values:

$$\langle z|Q|z\rangle = \sqrt{\frac{\hbar}{2m\omega}}\, \langle z|\left(a + a^{\dagger}\right)|z\rangle = \sqrt{\frac{2\hbar}{m\omega}}\,\mathrm{Re}\,z,$$
$$\langle z|P|z\rangle = \sqrt{2\hbar m\omega}\,\mathrm{Im}\,z, \tag{11.37}$$
$$\langle z|H|z\rangle = \hbar\omega\left(|z|^2 + \frac{1}{2}\right).$$

This is the classical result (11.30) if we ignore the zero-point energy $\hbar\omega/2$ in the expression for $\langle H\rangle$. Moreover, if the state of the harmonic oscillator is a coherent state at time $t = 0$, this property is conserved by the time evolution. Let us assume that the oscillator at time $t = 0$ is in the coherent state $|\varphi(t=0)\rangle = |z_0\rangle$ and calculate $|\varphi(t)\rangle$:

$$|\varphi(t)\rangle = e^{-iHt/\hbar}|z_0\rangle = e^{-i\omega t/2} e^{-i\omega N t}|z_0\rangle = e^{-i\omega t/2}|z_0 e^{-i\omega t}\rangle, \tag{11.38}$$

where we have used (11.35). We obtain the classical evolution $z(t) = z_0\exp(-i\omega t)$ up to a phase $\exp(-i\omega t/2)$ multiplying the state vector. If we start from a coherent state at time $t = 0$, the evolution of the expectation values $\langle Q\rangle$, $\langle P\rangle$, and $\langle H\rangle$ follows very exactly the classical evolution of $q(t)$, $p(t)$, and E. We have therefore shown that the expectation values in a coherent state obey the classical laws.

It is also instructive to calculate the dispersions. Let us evaluate, for example, $\langle Q^2\rangle$ in the coherent state $|z\rangle$:

$$\langle Q^2\rangle_z = \frac{\hbar}{2m\omega}\langle z|a^2 + (a^{\dagger})^2 + aa^{\dagger} + a^{\dagger}a|z\rangle = \frac{\hbar}{2m\omega}\langle z|a^2 + (a^{\dagger})^2 + 2a^{\dagger}a + 1|z\rangle$$
$$= \frac{\hbar}{2m\omega}\left[1 + (z + z^*)^2\right] = \frac{\hbar}{2m\omega}\left[1 + 4(\mathrm{Re}\,z)^2\right].$$

A similar calculation (Exercise 11.5.3) gives $\langle P^2\rangle$ and $\langle H^2\rangle$, from which we derive the dispersions[4] in the coherent state $|z\rangle$:

$$\boxed{\Delta_z Q = \sqrt{\frac{\hbar}{2m\omega}}, \quad \Delta_z P = \sqrt{\frac{m\hbar\omega}{2}}, \quad \Delta_z H = \hbar\omega|z|}\,. \tag{11.39}$$

The dispersion $\Delta_z H$ can be obtained from (11.34) using $\Delta H = \hbar\omega\Delta_z N$ and $\Delta_z N = \Delta n = |z|$, but it is also possible to calculate $\langle z|N^2|z\rangle$ directly. We note that the Heisenberg inequality is saturated in a coherent state: $\Delta_z Q\,\Delta_z P = \hbar/2$, and for $|z| \gg 1$

$$\frac{\Delta_z H}{\langle H\rangle} \simeq \frac{1}{|z|} \to 0 \ \text{ if } \ |z| \to \infty.$$

In summary, for $|z| \gg 1$ the dispersions about the expectation values are the smallest possible.

11.3 Introduction to quantized fields

11.3.1 Sound waves and phonons

When the vibration amplitudes are small, a system of coupled oscillators can be decomposed into normal modes and treated as a set of independent harmonic oscillators. An interesting case is that of vibrations in a solid, and we shall use it to introduce quantized fields. The first quantum model of vibrations in a crystalline solid was constructed by Einstein, who assumed that each atom can vibrate independently of the others about its equilibrium position with a frequency ω. In quantum physics each atom is therefore associated with a quantized harmonic oscillator of frequency ω. This model was the first to qualitatively explain the behavior of the specific heat of solids at low temperature: whereas the Dulong–Petit law predicts a specific heat independent of temperature, experiment shows that in fact this law is valid only at a sufficiently high temperature, and the specific heat actually decreases with temperature. However, the Einstein model does not give quantitatively correct results. This is not surprising, because the hypothesis of independent atomic vibrations is not realistic. If it were the case, vibrations would not be able to propagate in a solid and there would be no such thing as sound waves.

[4] We shall use either notation $(\Delta P, \Delta Q)$ or $(\Delta p, \Delta q)$ for the dispersions, as there is no possible ambiguity.

Let us study the simplest possible model of a chain of coupled oscillators, limiting ourselves to the case of one dimension. At equilibrium N atoms are located at regular intervals l along a line. The N equilibrium positions have abscissas $x_n = nl$, $n = 0, 1, \ldots, N-1$. It will be convenient to use periodic boundary conditions $x_{n+N} \equiv x_n$, but it is also possible to take vanishing ones: $x_0 = x_{N+1} = 0$. As before, we shall use q_n to denote the displacement from equilibrium of the nth atom. The coupling between the nth and $(n+1)$th atoms is described by the term $(K/2)(q_n - q_{n+1})^2$, where K is a constant, and the classical Hamiltonian of the ensemble is

$$\boxed{H_{\rm cl} = \sum_{n=0}^{N-1} \frac{p_n^2}{2m} + \frac{1}{2} K \sum_{n=0}^{N-1} (q_{n+1} - q_n)^2} \quad (11.40)$$

This is in fact the Hamiltonian of N identical masses m connected by identical springs with spring constant K (Fig. 11.1). In (11.40) $p_n = m\dot{q}_n$ is the momentum of the atoms. The first term in $H_{\rm cl}$ is the kinetic energy and the second is the potential energy. The equations of motion corresponding to the Hamiltonian (11.40) are written as

$$m\ddot{q}_n = -K\left[(q_n - q_{n-1}) + (q_n - q_{n+1})\right]. \quad (11.41)$$

Let us begin with the classical problem. To decouple the modes q_n, we seek the normal modes by taking the discrete (or lattice) Fourier transform of q_n and p_n:

$$q_k = \frac{1}{\sqrt{N}} \sum_{n=0}^{N-1} e^{ikx_n} q_n = \sum_n U_{kn} q_n, \quad k = j \times \frac{2\pi}{Nl}, \quad j = 0, \ldots, N-1. \quad (11.42)$$

To reduce the amount of notation we have not used $\tilde{q}_k$ to designate the Fourier transform, as the subscript k or n allows the Fourier components q_k and positions q_n on the lattice to be unambiguously distinguished. The matrix U_{kn} performs a discrete Fourier transform, and it is a unitary matrix:

$$\sum_n U_{kn} U^\dagger_{nk'} = \sum_n U_{kn} U^*_{k'n} = \frac{1}{N} \sum_n e^{ikx_n} e^{-ik'x_n} = \frac{1}{N} \sum_n \exp\left[\frac{2i\pi}{Nl}(j-j')x_n\right]$$
$$= \frac{1}{N} \frac{1 - \exp(2i\pi(j-j'))}{1 - \exp(2i\pi(j-j')/N)} = \delta_{jj'},$$

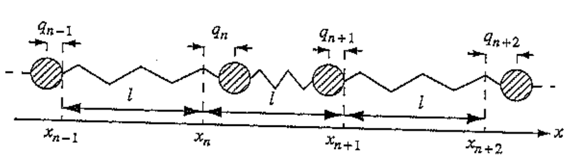

Fig. 11.1. Model for vibrations of a solid: a chain of springs.

that is, noting that $U^\dagger_{nk} = U^*_{kn} = U_{-kn}$,

$$\sum_n U_{kn} U^\dagger_{nk'} = \sum_n U_{kn} U_{-k'n} = \delta_{kk'}. \quad (11.43)$$

The range of variation of k is

$$0 \le k \le \frac{2\pi(N-1)}{Nl},$$

but, making use of the periodicity, we can replace this by the interval

$$-\frac{\pi}{l} \le k \le \frac{\pi}{l},$$

which is the first Brillouin zone already encountered in Section 9.5.2. Since we assume that $N \gg 1$, we neglect edge effects. The unitarity of the U_{kn} allows us to write down the inverse Fourier transform of (11.42):

$$q_n = \frac{1}{\sqrt{N}} \sum_{k=-\pi/l}^{\pi/l} e^{-ikx_n} q_k = \sum_k U^\dagger_{nk} q_k = \sum_k U_{-kn} q_k. \quad (11.44)$$

The Fourier transform (11.42) and its inverse (11.44) also apply to the momentum; we need only make the substitutions $q_n \to p_n$, $q_k \to p_k$. We obtain the desired expression for the Hamiltonian by expressing p_n and q_n as functions of p_k and q_k. The kinetic energy term is the simplest to evaluate:

$$\sum_n p_n^2 = \sum_n \sum_{k,k'} U_{-kn} U_{-k'n} p_k p_{k'} = \sum_{k,k'} \delta_{k,-k'}\, p_k p_{k'} = \sum_k p_k p_{-k}.$$

This is just the Parseval relation. Next we study the potential energy term:

$$\sum_n (q_{n+1} - q_n)^2 = \sum_n \sum_{k,k'} (e^{-ikl} - 1)(e^{-ik'l} - 1)\, U_{-kn} U_{-k'n} q_k q_{k'}$$
$$= \sum_k (e^{-ikl} - 1)(e^{ikl} - 1)\, q_k q_{-k} = 4 \sum_k \sin^2\left(\frac{kl}{2}\right) q_k q_{-k}.$$

Combining these two equations, we arrive at an expression for $H_{\rm cl}$ in which the modes are nearly decoupled:

$$H_{\rm cl} = \sum_k \frac{p_k p_{-k}}{2m} + \frac{1}{2} K \sum_k 4 \sin^2\left(\frac{kl}{2}\right) q_k q_{-k} = \sum_k \frac{p_k p_{-k}}{2m} + \frac{1}{2} m \sum_k \omega_k^2 q_k q_{-k}. \quad (11.45)$$

We have defined the frequency ω_k of the kth mode as

$$\omega_k = 2\sqrt{\frac{K}{m}} \sin\frac{|k|l}{2}. \quad (11.46)$$

The law (11.46) giving the frequency ω_k as a function of k is the *dispersion law* for the normal modes (Fig. 11.2). The expression (11.45) for $H_{\rm cl}$ as a function of the normal modes was obtained within the framework of classical physics. It can be generalized

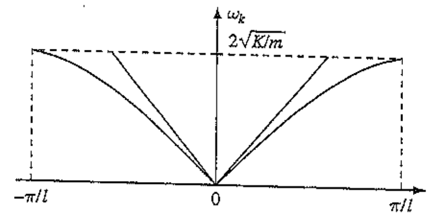

Fig. 11.2. Dispersion law of the normal modes.

immediately to the quantum version by replacing the numbers p_n and q_n in (11.40) by the operators P_n and Q_n obeying the commutation relations

$$[Q_n, P_{n'}] = i\hbar\delta_{nn'}I, \tag{11.47}$$

because the operators corresponding to different atoms n and n' commute. The Fourier transforms can be carried over without modification to the quantum version of the problem, and we obtain

$$H = \sum_k \frac{P_k P_{-k}}{2m} + \frac{1}{2}K\sum_k 4\sin^2\left(\frac{kl}{2}\right) Q_k Q_{-k} = \sum_k \frac{P_k P_{-k}}{2m} + \frac{1}{2}m\sum_k \omega_k^2 Q_k Q_{-k}.$$

The commutation relations of the Q_k and P_k are

$$[Q_k, P_{k'}] = \sum_{nn'} U_{kn}U_{k'n'}[Q_n, P_{n'}] = i\hbar I\sum_n U_{kn}U_{k'n} = i\hbar\,\delta_{k,-k'}I. \tag{11.48}$$

We still need to decouple the modes k and $-k$. To do this we introduce the annihilation and creation operators of the normal modes by analogy with (11.4) and (11.6)–(11.7):

$$Q_k = \sqrt{\frac{\hbar}{2m\omega_k}}\,(a_k + a_{-k}^\dagger)\,, \quad P_k = \frac{1}{i}\sqrt{\frac{\hbar m\omega_k}{2}}\,(a_k - a_{-k}^\dagger)\,. \tag{11.49}$$

It can immediately be verified that the commutation relations (11.48) are satisfied when[5]

$$\boxed{[a_k, a_{k'}^\dagger] = \delta_{kk'}I}\,. \tag{11.50}$$

The factors $\delta_{k,-k'}$ in (11.48) and $\delta_{kk'}$ in (11.50) should be noted. They originate in the periodic boundary conditions, which imply plane waves with $k > 0$ and $k < 0$. If vanishing boundary conditions are used, we have only $k > 0$ and we find the factor $\delta_{kk'}$;

[5] Equivalently, a_k and $a_k^\dagger$ can be expressed as functions of Q_k and P_k and then the commutation relations (11.50) derived.

see Exercise 11.5.9. Substituting the relations (11.49) into the expression for H and using the commutation relations (11.50), we arrive at the final form of H:

$$\boxed{H = \sum_{k=-\pi/l}^{\pi/l} \hbar\omega_k\left(a_k^\dagger a_k + \frac{1}{2}\right)}\,. \tag{11.51}$$

The Hamiltonian is a sum of independent harmonic oscillators of frequency ω_k. Let $|r\rangle$ be an eigenstate of H, $H|r\rangle = E_r|r\rangle$. Using the commutation relations (11.11), we have

$$Ha_k|r\rangle = (a_k H + [H, a_k])\,|r\rangle = (E_r - \hbar\omega_k)a_k|r\rangle,$$
$$Ha_k^\dagger|r\rangle = (a_k^\dagger H + [H, a_k^\dagger])\,|r\rangle = (E_r + \hbar\omega_k)a_k^\dagger|r\rangle.$$

The creation operator $a_k^\dagger$ *increases* the energy by $\hbar\omega_k$, and the annihilation operator a_k *decreases* it by $\hbar\omega_k$. This energy is associated with an *elementary excitation* or a *quasi-particle*, called a *phonon*. The operator $N_k = a_k^\dagger a_k$, which commutes with H, counts the number of phonons in the mode k. Let $|0_k\rangle$ be the ground state of the kth mode: $a_k|0_k\rangle = 0$. This state corresponds to zero phonons in the kth mode. Let us construct the state $|n_k\rangle$ containing n_k phonons in the kth mode using (11.18):

$$|n_k\rangle = \frac{1}{\sqrt{n_k!}}\,(a_k^\dagger)^{n_k}|0_k\rangle, \tag{11.52}$$

and the eigenstates of H by forming the tensor product of the states $|n_k\rangle$:

$$|r\rangle = \bigotimes_{k=-\pi/l}^{k=\pi/l}|n_k\rangle, \tag{11.53}$$

$$H|r\rangle = \sum_{k=-\pi/l}^{\pi/l}\left(n_k + \frac{1}{2}\right)\hbar\omega_k|r\rangle. \tag{11.54}$$

The Hilbert space thus constructed is called the *Fock space*. The state $|r\rangle$ is specified by its *occupation numbers* n_k, or the number of phonons in the kth mode. The formalism that we have developed allows us to describe situations in which the number of particles is variable; in fact, we have just constructed a quantized field using the simplest possible nontrivial example.

11.3.2 *Quantization of a scalar field in one dimension*

Now that we have quantized elasticity, our objective is to do the same with the electromagnetic field. We shall pass through an intermediate stage where we quantize a simple model, that of the *scalar field* in one dimension, which we define below. This model is relevant to the physical case of vibrations of an elastic rod considered as a continuous medium. When $|k|l \ll 1$, the dispersion law (11.46) becomes linear in $|k|$:

$$|k|l \ll 1 : \omega_k \simeq \sqrt{\frac{K}{m}}\,|k|l = c_s|k|, \tag{11.55}$$

where $c_s = l\sqrt{K/m}$ is the speed of sound at low frequencies. It will prove useful to rewrite this equation as a relation between the speed of sound, Young's modulus $Y = Kl$,[6] and the mass per unit length $\mu = m/l$:

$$c_s = \sqrt{\frac{Y}{\mu}}. \tag{11.56}$$

Our scalar field will be the long-wavelength limit $\lambda \gg l$ (or $|k|l \ll 1$) of the lattice model of the preceding subsection, and the linear dispersion law (11.55) $\omega_k = c_s|k|$ will be assumed valid for all k. In fact, our ultimate goal is to take the limit $l \to 0$, also called the *continuum limit* of the lattice model. We introduce two functions $\varphi(x, t)$ and $\pi(x, t)$ such that

$$q_n(t) = \varphi(x_n, t), \quad p_n(t) = l\pi(x_n, t). \tag{11.57}$$

In the long-wavelength limit, the displacements $q_n(t)$ and momenta $p_n(t)$ vary only slightly from one site to another, and so we can use the following approximation for the derivative of $\varphi(x, t)$ with respect to x:

$$\left.\frac{\partial\varphi}{\partial x}\right|_{x=x_n} \simeq \frac{1}{l}\left[\varphi(x_{n+1}, t) - \varphi(x_n, t)\right] = \frac{1}{l}\left[q_{n+1}(t) - q_n(t)\right]. \tag{11.58}$$

The equation of motion (11.41) becomes

$$\mu\left.\frac{\partial^2\varphi}{\partial t^2}\right|_{x=x_n} = \frac{Y}{l^2}\Big\{[\varphi(x_{n+1}) - \varphi(x_n)] + [\varphi(x_{n-1}) - \varphi(x_n)]\Big\}.$$

A Taylor series expansion through order l^2 gives

$$\varphi(x+l) + \varphi(x-l) - 2\varphi(x) \simeq l^2\frac{\partial^2\varphi}{\partial x^2},$$

and we obtain a wave equation describing the propagation of vibrations at speed c_s:

$$\frac{\partial^2\varphi}{\partial t^2} - c_s^2\frac{\partial^2\varphi}{\partial x^2} = 0. \tag{11.59}$$

The classical Hamiltonian is written as a function of φ_n and π_n as

$$H_{\rm cl} = l\sum_n\left\{\frac{\pi^2(x_n)}{2\mu} + \frac{1}{2}Kl\left[\frac{\varphi(x_{n+1}) - \varphi(x_n)}{l}\right]^2\right\},$$

[6] In one dimension, the change of length ΔL of a rod of length L acted on by a force $F = K\Delta x$ satisfies

$$\frac{\Delta L}{L} = \frac{F}{Y} = \frac{\Delta x}{l} = \frac{F}{Kl},$$

which gives $Y = Kl$. In three dimensions $\Delta L/L = F/YS$, where S is the cross-sectional area of the rod and $Y = K/l$. $c_s = \sqrt{Y/\mu}$ with $\mu = m/l^3$.

which is an approximation to the integral

$$\boxed{H_{\rm cl} = \int_0^L \mathrm{d}x\left[\frac{1}{2\mu}\pi^2(x) + \frac{1}{2}\mu c_s^2\left(\frac{\partial\varphi}{\partial x}\right)^2\right]}, \tag{11.60}$$

where $L = Nl$ is the length of the rod: $H_{\rm cl}$ in (11.60) is the continuum version of (11.40).[7] We have suppressed the time dependence: $\varphi(x) = \varphi(x, t = 0)$ and $\pi(x) = \pi(x, t = 0)$ because $H_{\rm cl}$ is independent of time.

As in the preceding subsection, we shall decompose $\varphi(x)$ and $\pi(x)$ into normal modes by means of a Fourier transform. We define φ_k as

$$\varphi_k = \varphi^*_{-k} = \frac{1}{\sqrt{L}}\int_0^L \mathrm{d}x\,\mathrm{e}^{\mathrm{i}kx}\,\varphi(x) \simeq \frac{l}{\sqrt{Nl}}\sum_n \mathrm{e}^{\mathrm{i}kx_n}\varphi(x_n) = \sqrt{l}\,q_k \tag{11.61}$$

by comparison with (11.42). The inverse of φ_k is given by

$$\varphi(x) = \frac{1}{\sqrt{L}}\sum_k \mathrm{e}^{-\mathrm{i}kx}\,\varphi_k. \tag{11.62}$$

The relation for p_k corresponding to (11.83) is $\pi_k = l^{-1/2}p_k$. Now let us go to the quantum version, replacing the numbers φ_k and π_k by the *operators* Φ_k and Π_k obeying commutation relations derived from (11.48):[8]

$$[\Phi_k, \Pi_{k'}] = \mathrm{i}\hbar\delta_{k,-k'}I. \tag{11.63}$$

As a consequence, if the numbers φ_k and π_k in (11.62) and in the corresponding equation for $\pi(x)$ are replaced by the operators Φ_k and Π_k, the functions $\varphi(x)$ and $\pi(x)$ become operators $\Phi(x)$ and $\Pi(x)$. Here $\Phi(x)$ is called a *field operator* or a *quantized field*.[9] We note that $\Phi(x, t)$ and $\Pi(x, t)$ are labeled by a continuous variable x, whereas their Fourier transforms Φ_k and Π_k are labeled by a discrete index k. This property follows from the use of boundary conditions in a box: $0 \le x \le L$. The variable x is *not* a dynamical variable which is transformed into an operator in the quantum version of the problem, but rather the *label* of a point on the rod, and the fundamental operators are Φ and Π.

[7] The reader familiar with analytical mechanics will note that the Hamilton equations are

$$\frac{\delta H}{\delta\pi(x)} = \frac{1}{\mu}\pi = \dot\varphi, \quad \frac{\delta H}{\delta\varphi(x)} = -Y\frac{\partial^2\varphi}{\partial x^2} = -\mu\ddot\varphi,$$

which give the wave equation (11.59).

[8] The usual procedure is to derive these relations from the equal-time canonical commutation relations postulated between the field $\Phi(x, t)$ and its "conjugate momentum" $\Pi(x, t)$:

$$[\Phi(x, t), \Pi(x', t)] = \mathrm{i}\hbar\delta(x - x')I,$$

which will be demonstrated below in (11.69) starting from (11.63). This procedure is – mistakenly – considered by some authors to be more "rigorous"; in fact, it is just as heuristic as the one we follow here.

[9] The procedure we have followed is sometimes called "second quantization." This expression is completely misleading. Clearly, there is only a single quantization, and so "second quantization" should definitively be banished.

Now we can express the quantum Hamiltonian H as a function of the Fourier components of Π and Φ. We write, for example, the potential energy term as a function of the Φ_k as

$$\int_0^L \mathrm{d}x \left(\frac{\partial\Phi}{\partial x}\right)^2 = \frac{1}{L}\int \mathrm{d}x \sum_{k,k'} \Phi_k\Phi_{k'}(-\mathrm{i}k)(-\mathrm{i}k')\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{e}^{-\mathrm{i}k'x}$$
$$= -\sum_k \Phi_k\Phi_{k'}kk'\delta_{k,-k'} = \sum_k k^2\Phi_k\Phi_{-k}.$$

This leads to the following expression for the quantum Hamiltonian H:

$$H = \sum_k \left(\frac{1}{2\mu}\Pi_k\Pi_{-k} + \frac{1}{2}\mu\, c_s^2k^2\Phi_k\Phi_{-k}\right). \tag{11.64}$$

Finally, as in (11.49), we introduce the operators a_k and $a_k^\dagger$ satisfying the commutation relations (11.50):

$$\Phi_k = \sqrt{\frac{\hbar}{2\mu\omega_k}}\,(a_k + a_{-k}^\dagger), \quad \Pi_k = \frac{1}{\mathrm{i}}\sqrt{\frac{\hbar\mu\omega_k}{2}}\,(a_k - a_{-k}^\dagger), \tag{11.65}$$

and H again takes the form of a sum of independent harmonic oscillators:

$$H = \sum_k \hbar\omega_k\left(a_k^\dagger a_k + \frac{1}{2}\right). \tag{11.66}$$

The result is superficially identical to (11.51), but there is an essential difference. The earlier wave vectors k were bounded as $|k| \le \pi/l$. Now in the continuum limit there is no longer a bound on k and the zero-point energy

$$E_0 = \sum_k \frac{1}{2}\hbar\omega_k$$

is infinite. However, this infinite result is artificial in this particular case (Exercise 11.5.6). Actually, when the wave vector k becomes large or, equivalently, when the wavelength $\lambda = 2\pi/k$ becomes small, of the order of the lattice spacing l, the continuum theory is no longer valid. It is only when the wavelength of a vibration satisfies $\lambda \gg l$ that the wave does not "see" the underlying crystal lattice. We shall encounter this problem of infinite energy again in the case of the electromagnetic field, where k will be genuinely unbounded.

Let us conclude this subsection by giving the Fourier expansion of the quantized field $\Phi_{\mathrm{H}}(x,t)$ in the Heisenberg picture (4.31), with $\Phi_{\mathrm{H}}(x,t=0) = \Phi_S(x) = \Phi(x)$. The time dependence is found using the equations

$$a_k(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar}\,a_k\,\mathrm{e}^{-\mathrm{i}Ht/\hbar} = a_k\,\mathrm{e}^{-\mathrm{i}\omega_k t},$$
$$a_k^\dagger(t) = \mathrm{e}^{\mathrm{i}Ht/\hbar}\,a_k^\dagger\,\mathrm{e}^{-\mathrm{i}Ht/\hbar} = a_k^\dagger\,\mathrm{e}^{-\mathrm{i}\omega_k t}, \tag{11.67}$$

which follow from

$$\frac{\mathrm{d}a_k}{\mathrm{d}t} = -\mathrm{i}[a_k(t), H] = -\mathrm{i}\omega_k a_k(t),$$

and we obtain from (11.62) and (11.65)

$$\boxed{\Phi_{\mathrm{H}}(x,t) = \sqrt{\frac{\hbar}{2\mu L}}\sum_k \frac{1}{\sqrt{\omega_k}}\left[a_k\mathrm{e}^{\mathrm{i}(kx-\mathrm{i}\omega_k t)} + a_k^\dagger\mathrm{e}^{-\mathrm{i}(kx-\mathrm{i}\omega_k t)}\right]}\,. \tag{11.68}$$

We check from this expression that the field operator $\Phi_{\mathrm{H}}(x,t)$ (which has the dimensions of a length) is Hermitian as it should be. The commutation relations of $\Phi_{\mathrm{H}}(x,t)$ and $\Pi_{\mathrm{H}}(x',t)$ can be calculated immediately. First we take $t=0$, $\Phi(x) = \Phi_{\mathrm{H}}(x,t=0)$, $\Pi(x') = \Pi_{\mathrm{H}}(x',t=0)$:

$$[\Phi(x), \Pi(x')] = -\frac{\mathrm{i}\hbar}{2L}\sum_{k,k'}\sqrt{\frac{\omega_{k'}}{\omega_k}}\left[a_k\,\mathrm{e}^{\mathrm{i}kx} + a_k^\dagger\,\mathrm{e}^{-\mathrm{i}kx},\, a_{k'}\,\mathrm{e}^{\mathrm{i}k'x} - a_{k'}^\dagger\,\mathrm{e}^{-\mathrm{i}k'x}\right]$$
$$= \frac{\mathrm{i}\hbar}{L}\sum_k \mathrm{e}^{\mathrm{i}k(x-x')}I = \mathrm{i}\hbar\delta(x-x')I, \tag{11.69}$$

where we have used (9.145) to obtain the last expression. Since this commutator is a multiple of the identity, we trivially obtain the same result for the equal-time commutator $[\Phi_{\mathrm{H}}(x,t), \Pi_{\mathrm{H}}(x',t)]$.

11.3.3 Quantization of the electromagnetic field

The quantization of the electromagnetic field follows that of the scalar field in the preceding subsection with three modifications: we must work in three dimensions, we must take into account the vector nature of the electromagnetic field, and we must replace the speed of sound c_s by the speed of light c. Let us recall the Maxwell equations (1.8)–(1.9) for electric field $\vec{E}$ and magnetic field $\vec{B}$:

$$\vec{\nabla}\cdot\vec{B} = 0, \qquad \vec{\nabla}\times\vec{E} = -\frac{\partial\vec{B}}{\partial t}, \tag{11.70}$$

$$\vec{\nabla}\cdot\vec{E} = \frac{\rho_{\mathrm{em}}}{\varepsilon_0}, \quad c^2\vec{\nabla}\times\vec{B} = \frac{\partial\vec{E}}{\partial t} + \frac{1}{\varepsilon_0}\vec{j}_{\mathrm{em}}. \tag{11.71}$$

The two equations (11.70) are *constraints* on the fields $\vec{E}$ and $\vec{B}$, and the two equations (11.71) depend on the *sources* of the electromagnetic field, that is, the charge density ρ_{em} and the current density $\vec{j}_{\mathrm{em}}$. From the Maxwell equations we can derive the continuity equation:

$$\frac{\partial\rho_{\mathrm{em}}}{\partial t} + \vec{\nabla}\cdot\vec{j}_{\mathrm{em}} = 0. \tag{11.72}$$

One could dream of quantizing the fields $\vec{E}$ and $\vec{B}$ directly. However, there are two technical difficulties with this. First, $\vec{E}$ and $\vec{B}$ are related by the constraints (11.70), which means that their six components are not independent and, moreover, as shown by the

Bohm–Aharonov effect,[10] the interaction of the electromagnetic field with the charges is not local. It is preferable to use the intermediary of the scalar and vector potentials[11] $\overline{V}$ and $\vec{A}$ and obtain the fields by partial differentiation:

$$\vec{E} = -\vec{\nabla}\overline{V} - \frac{\partial \vec{A}}{\partial t}, \quad \vec{B} = \vec{\nabla}\times\vec{A}. \tag{11.73}$$

The use of potentials instead of fields should not be surprising; in quantum mechanics we have never used forces, which are related directly to the fields $\vec{E}$ and $\vec{B}$ by the Lorentz law (1.11); instead, we used the potential energy. In quantum mechanics it is the energy and momentum that play the fundamental role, because they directly influence the phase of the wave function. In the presence of an electric field $\vec{E}$, it is the potential $\overline{V}$ that shows up in the Schrödinger equation via the potential energy $V = q\overline{V}$. It is therefore not surprising that in the presence of a magnetic field $\vec{B}$, it is the vector potential $\vec{A}$ that is involved directly in the Schrödinger equation rather than the field $\vec{B}$.

The potentials are not unique. Under a *gauge transformation*

$$\boxed{\vec{A} \to \vec{A}' = \vec{A} - \vec{\nabla}\Lambda, \quad \overline{V} \to \overline{V}' = \overline{V} + \frac{\partial \Lambda}{\partial t}}, \tag{11.74}$$

where $\Lambda(\vec{r}, t)$ is a scalar function of space and time, the fields $\vec{E}$ and $\vec{B}$ are unchanged. To eliminate this arbitrariness in the potentials $(\vec{A}, \overline{V})$, it is usual to choose a gauge by imposing a condition on $(\vec{A}, \overline{V})$. A common choice (but not the only one possible!) which we shall use here is the *Coulomb gauge*, or the *radiation gauge*:

$$\boxed{\vec{\nabla}\cdot\vec{A} = 0}. \tag{11.75}$$

With this choice, the vector potential becomes transverse: in Fourier space, the condition (11.75) becomes $\vec{k}\cdot\vec{A}(\vec{k}) = 0$ (see also Exercise 11.5.7). According to the first equation in (11.71) and (11.73),

$$\vec{\nabla}\cdot\left(\vec{\nabla}\overline{V} + \frac{\partial \vec{A}}{\partial t}\right) = \nabla^2\overline{V} + \frac{\partial}{\partial t}(\vec{\nabla}\cdot\vec{A}) = \nabla^2\overline{V} = -\frac{\rho_{\rm em}}{\varepsilon_0},$$

from which we derive the scalar potential $\overline{V}$:

$$\overline{V}(\vec{r}, t) = \frac{1}{4\pi\varepsilon_0}\int \frac{\rho_{\rm em}(\vec{r}', t)}{|\vec{r}-\vec{r}'|}\,{\rm d}^3r'. \tag{11.76}$$

This expression for the scalar potential is called the *instantaneous Coulomb potential*, because the retardation effects are not explicit: the time t in $\overline{V}$ is the same as that of the source $\rho_{\rm em}$. This might seem to be incompatible with relativity, but it should be born in mind that a potential is not directly observable, and so the contradiction is only apparent.[12]

[10] See, for example, Feynman *et al.* [1965], Vol. II, Chapter 15.
[11] We use the notation $\overline{V}$ for the electric potential so as not to create confusion with the potential energy V. A particle of charge q in a potential $\overline{V}$ has potential energy $V = q\overline{V}$.
[12] Cf. Weinberg [1995], Chapter 8.

In the absence of sources, $\rho_{\rm em} = \vec{j}_{\rm em} = 0$, the second of Equations (11.71) is written as

$$c^2\vec{\nabla}\times(\vec{\nabla}\times\vec{A}) = c^2\vec{\nabla}\cdot(\vec{\nabla}\cdot\vec{A}) - c^2\nabla^2\vec{A} = -\frac{\partial(\vec{\nabla}\overline{V})}{\partial t} - \frac{\partial^2\vec{A}}{\partial t^2},$$

or, using (11.75) and the fact that $\overline{V} = 0$,

$$\frac{\partial^2\vec{A}}{\partial t^2} - c^2\nabla^2\vec{A} = 0. \tag{11.77}$$

This wave equation is analogous to (11.59) with the three following differences: (i) the spatial dimension is three rather than one; (ii) it involves the speed of light c rather than the speed of sound c_s; (iii) the field $\vec{A}$ is a vector field and not a scalar one. Using the classical expression for the energy density of the electromagnetic field, the expression for the classical Hamiltonian becomes

$$H_{\rm cl} = \frac{1}{2}\varepsilon_0\int {\rm d}^3r\left(\vec{E}^2 + c^2\vec{B}^2\right). \tag{11.78}$$

If $\vec{A}$ is the analog of φ, then $\vec{E} = -\partial\vec{A}/\partial t$ will be the analog[13] of π and the term $c^2\vec{B}^2$, which depends on spatial derivatives of $\vec{A}$, will be the analog of $c_s^2(\partial\varphi/\partial x)^2$. We can immediately write down a Fourier expansion for the quantized electromagnetic field $\vec{\mathsf{A}}_{\rm H}(\vec{r}, t)$ by analogy with (11.68),[14] making the replacements $L \to L^3$ and $\mu \to \varepsilon_0$. The last substitution is determined by comparing the terms $\varepsilon_0 c^2(\vec{\nabla}\times\vec{A})^2$ in (11.78) and $\mu c_s^2(\partial\varphi/\partial x)^2$ in (11.60). The final difference from (11.68) is that $\vec{\mathsf{A}}$ is a vector. A priori, a Fourier component of $\vec{\mathsf{A}}$ should be decomposed on an orthonormal basis of three unit vectors $\hat{k}$, $\vec{e}_1(\hat{k})$, and $\vec{e}_2(\hat{k})$ with $\hat{k}\cdot\vec{e}_i(\hat{k}) = 0$. This is effectively the case for sound vibrations in three dimensions in an isotropic medium,[15] where the vibrations can be either compression waves, which are longitudinal waves parallel to $\hat{k}$, or shear waves, which are transverse and perpendicular to $\hat{k}$. In the case of an electromagnetic field, the gauge condition (11.75) becomes $\hat{k}\cdot\vec{\mathsf{A}}(\vec{k}) = 0$ in Fourier space and there is no longitudinal component. Taking into account all these considerations, we can generalize (11.68) and write the quantized electromagnetic field[16] in the Heisenberg picture (we continue to use periodic boundary conditions in a box of volume $\mathcal{V} = L^3$, or *quantization in a box*):

$$\boxed{\vec{\mathsf{A}}_{\rm H}(\vec{r}, t) = \sqrt{\frac{\hbar}{2\varepsilon_0 L^3}}\sum_{\vec{k}}\sum_{s=1}^{2}\frac{1}{\sqrt{\omega_k}}\left[a_{\vec{k}s}\vec{e}_s(\hat{k}){\rm e}^{{\rm i}(\vec{k}\cdot\vec{r}-\omega_k t)} + a^\dagger_{\vec{k}s}\vec{e}^{\,*}_s(\hat{k}){\rm e}^{-{\rm i}(\vec{k}\cdot\vec{r}-\omega_k t)}\right]}. \tag{11.79}$$

[13] In fact, in a formulation of electromagnetism like that used in analytical mechanics (cf. Footnote 7), it is $-\varepsilon_0\vec{E}$ that plays the role of the momentum conjugate to $\vec{A}$, as seen from (11.85).
[14] In order to distinguish quantized fields from classical ones, we shall designate the former by sans serif letters: $\vec{\mathsf{A}}$, $\vec{\mathsf{E}}$, $\vec{\mathsf{B}}$.
[15] Our discussion is actually oversimplified, because the speed of compression waves is different from that of shear waves.
[16] We have glossed over several delicate problems; see, for example, Weinberg [1995], Chapter 8, for a full discussion.

The unit vectors $\vec{e}_s(\hat{k})$ orthogonal to $\vec{k}$ describe the polarization. It is possible to choose a complex polarization basis, for example, a basis of circular polarization states: $s = \mathrm{R}, \mathrm{L}$, which makes it necessary to perform the complex conjugation in the second term of (11.79), thus ensuring that $\vec{\mathsf{A}}$ is Hermitian. The expression for the projector onto the subspace orthogonal to $\vec{k}$ is often useful:

$$\sum_s e_{si}(\hat{k})\, e^*_{sj}(\hat{k}) = \delta_{ij} - \hat{k}_i\hat{k}_j. \tag{11.80}$$

The operators $a_{\vec{k}s}$ ($a^\dagger_{\vec{k}s}$) destroy (create) photons of wave vector $\vec{k}$ and polarization s. They satisfy the commutation relations

$$\boxed{[a_{\vec{k}s}, a^\dagger_{\vec{k}'s'}] = \delta_{\vec{k},\vec{k}'}\delta_{ss'}I}\ . \tag{11.81}$$

From (11.79) we derive the expression for the quantized electric field $\vec{\mathsf{E}}_\mathrm{H} = -\partial\vec{\mathsf{A}}_\mathrm{H}/\partial t$:

$$\vec{\mathsf{E}}_\mathrm{H}(\vec{r}, t) = \mathrm{i}\sqrt{\frac{\hbar}{2\varepsilon_0 L^3}}\sum_{\vec{k}}\sum_{s=1}^{2}\sqrt{\omega_k}\left[a_{\vec{k}s}\vec{e}_s(\hat{k})\mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{r}-\omega_k t)} - a^\dagger_{\vec{k}s}\vec{e}^{\,*}_s(\hat{k})\mathrm{e}^{-\mathrm{i}(\vec{k}\cdot\vec{r}-\omega_k t)}\right] \tag{11.82}$$

and, using the expression

$$\vec{\nabla}\times\left(\vec{e}_s(\hat{k})\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}}\right) = \mathrm{i}\vec{k}\times\vec{e}_s(\hat{k})\,\mathrm{e}^{\mathrm{i}\vec{k}\cdot\vec{r}}, \tag{11.83}$$

that for the magnetic field:

$$\vec{\mathsf{B}}_\mathrm{H}(\vec{r}, t) = \sqrt{\frac{\hbar}{2\varepsilon_0 L^3}}\sum_{\vec{k}}\sum_{s=1}^{2}\frac{\mathrm{i}}{c}\sqrt{\omega_k}\,\hat{k}\times\left[\vec{e}_s(\hat{k})a_{\vec{k}s}\mathrm{e}^{\mathrm{i}(\vec{k}\cdot\vec{r}-\omega_k t)} - \vec{e}^{\,*}_s(\hat{k})a^\dagger_{\vec{k}s}\mathrm{e}^{-\mathrm{i}(\vec{k}\cdot\vec{r}-\omega_k t)}\right]. \tag{11.84}$$

Just like for a classical plane wave, $\vec{\mathsf{B}} = (\hat{k}/c)\times\vec{\mathsf{E}}$. It is easy, as in the case of a scalar field, to calculate the commutators of the various components of the field at $t = 0$. We then find the following commutation relations between the field component A_i and the component $-\varepsilon_0\mathsf{E}_j$ of the conjugate momentum (Exercise 11.5.8):

$$[\mathsf{A}_i(\vec{r}), -\varepsilon_0\mathsf{E}_j(\vec{r}\,')] = \mathrm{i}\hbar\int\frac{\mathrm{d}^3k}{(2\pi)^3}\,\mathrm{e}^{\mathrm{i}\vec{k}\cdot(\vec{r}-\vec{r}\,')}\left(\delta_{ij} - \hat{k}_i\hat{k}_j\right)I, \tag{11.85}$$

where we have used (9.151). We then deduce that E_x commutes with B_x, but not with B_y or B_z, which shows that it is not possible to measure simultaneously the x component of the electric field and the y component of the magnetic field at the same point.

The expression for the Hamiltonian (Exercise 11.5.8) is a trivial generalization of (11.66):

$$\boxed{H = \sum_{\vec{k},s}\hbar\omega_k\left(a^\dagger_{\vec{k},s}a_{\vec{k},s} + \frac{1}{2}\right)}\ . \tag{11.86}$$

We then find the (infinite) zero-point energy:

$$E_0 = \frac{1}{2}\sum_{\vec{k},s}\hbar\omega_k \to \frac{L^3}{(2\pi)^3}\int\mathrm{d}^3k\,\hbar ck = \frac{\hbar c L^3}{2\pi^2}\int_0^\infty k^3\mathrm{d}k, \tag{11.87}$$

where we have used (9.151). In the case of black-body radiation, it was shown that the thermal fluctuations leading to infinite energy in classical statistical mechanics can be controlled by quantum mechanics. However, we eliminated that infinity by introducing another one, an infinity associated with *quantum fluctuations*. These quantum fluctuations have observable effects: for example, they lead to the Casimir effect (Exercise 11.5.12). The zero-point energy is also called the *vacuum energy*; it may play an important role in cosmology, where it might be related to the so-called dark energy, whose properties are still far from being understood.

It is possible to couple the quantized field to a classical source $\vec{\jmath}_\mathrm{em}(\vec{r}, t)$ by writing

$$W(t) = -\int\mathrm{d}^3r\,\vec{\jmath}_\mathrm{em}(\vec{r}, t)\cdot\vec{\mathsf{A}}(\vec{r}). \tag{11.88}$$

This coupling generalizes that of (11.124) for the forced harmonic oscillator of Exercise 11.5.4, with the force $f(t)$ replaced by the source $\vec{\jmath}_\mathrm{em}$ and the position operator Q replaced by the quantized field $\vec{\mathsf{A}}$. It can then be shown[17] that if we start from a state with zero photons and if the source acts for a finite time, we obtain a coherent state of the electromagnetic field in which the number of photons in a mode $\vec{k}$ obeys a Poisson law with average given by $|\vec{\jmath}_\mathrm{em}(\vec{k}, \omega_k)|^2$, where $\vec{\jmath}_\mathrm{em}(\vec{k}, \omega_k)$ is the four-dimensional Fourier transform of $\vec{\jmath}_\mathrm{em}(\vec{r}, t)$.

The quantized field $\vec{\mathsf{A}}$ was written down in the Coulomb gauge. This is the gauge most convenient for elementary problems, but it is not convenient for a general study of quantum electrodynamics. The condition $\vec{\nabla}\cdot\vec{\mathsf{A}} = 0$ distinguishes a particular reference frame, and so the Lorentz invariance of the theory is not manifest. Naturally, this is not a fundamental defect, because it is possible to show that the physical results are consistent with Lorentz invariance. The real fault of the Coulomb gauge is that it leads to inextricable calculations because the renormalization procedure (elimination of infinities) requires that Lorentz invariance be maintained explicitly in order for the calculations to be manageable.[18] A gauge in which Lorentz invariance is manifest is the Lorentz gauge:[19]

$$\frac{\partial\overline{V}}{\partial t} + \vec{\nabla}\cdot\vec{A} = 0.$$

However, the Lorentz gauge introduces unphysical states, which must be correctly interpreted and eliminated from the physical results. These unphysical states do not appear in the Coulomb gauge, which is an example of a "physical gauge." Unfortunately, it is not possible to use a physical gauge and preserve formal Lorentz invariance at the same time.

[17] See Exercise 11.5.4. A detailed discussion can be found, for example, in Le Bellac [1991], Chapter 9, or C. Itzykson and J.-B. Zuber, *Quantum Field Theory*, New York: McGraw-Hill (1980), Chapter 4.

[18] From a technical point of view, the counter-terms that eliminate the infinities are constrained by the Lorentz invariance if the gauge choice respects this formal invariance.

[19] This formal Lorentz invariance is manifest in four-dimensional notation: $\partial_\mu A^\mu = 0$, $A^\mu = (\overline{V}, \vec{A})$.