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Discrete Systems

1.1 One-Dimensional Harmonic Crystal

We begin with the quantum mechanics of a vibrating crystal. To the naked eye the crystal appears to be a continuous elastic solid. We know, however, that, when viewed through a sufficiently powerful microscope it will be revealed to be composed of individual atoms held together by chemical bonds. For our purpose the atoms and bonds can be thought of as “balls and springs,” and the crystal as an assembly of coupled harmonic oscillators. If you understand the quantum mechanics of harmonic oscillators, it will not be difficult to apply this understanding to study the effectively continuous crystal. This is our task in this chapter.

1.1.1 Normal Modes

To avoid the complexities of real crystals with their plethora of elastic constants and modes, we will consider a simple one-dimensional model of a crystal.

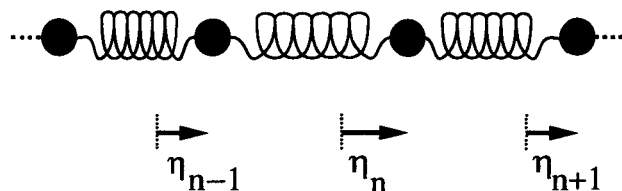


Fig 1. A one-dimensional crystal.

We will take a line of atoms of unit mass whose equilibrium positions are at a set of sites on the x axis labeled by the integer n , and separated by a distance a . We will assume the atoms are free to vibrate only in the x direction, so we are dealing with longitudinal waves, and denote the displacement of the atom at site n by η_n .

The quickest route to the dynamics uses the lagrangian. As always in mechanics this is the difference of the kinetic energy T and the potential energy V . For a *harmonic crystal* V is a sum of terms of the form $\frac{1}{2}\lambda(\eta_n - \eta_{n+1})^2$, where λ is the spring constant. Thus

$$L = T - V = \sum_n \left\{ \frac{1}{2} \dot{\eta}_n^2 - \frac{\lambda}{2} (\eta_n - \eta_{n+1})^2 \right\}. \quad (1.1)$$

From Lagrange's equations, one for each η_n ,

$$\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{\eta}_n} \right) - \frac{\partial L}{\partial \eta_n} = 0, \quad (1.2)$$

we find the classical equations of motion

$$\ddot{\eta}_n = \lambda(\eta_{n+1} + \eta_{n-1} - 2\eta_n). \quad (1.3)$$

These have solutions in the form of complex traveling waves

$$\eta_n = e^{ikn - i\omega t}, \quad (1.4)$$

where

$$\omega^2 = 2\lambda(1 - \cos k). \quad (1.5)$$

In the long-wavelength limit $k \ll 1$, this dispersion relation reduces to

$$\omega^2 = \lambda k^2, \quad (1.6)$$

which means that the long-wavelength sound waves have velocity $\sqrt{\lambda}$.

In the next chapter we will have cause to consider an additional term in the lagrangian, which corresponds to a harmonic potential $\frac{1}{2}\Omega^2\eta_n^2$ pinning each of the particles to the vicinity of its initial location. Including this, L becomes

$$L = \sum_n \left\{ \frac{1}{2} \dot{\eta}_n^2 - \frac{\lambda}{2} (\eta_n - \eta_{n+1})^2 - \frac{1}{2} \Omega^2 \eta_n^2 \right\}. \quad (1.7)$$

The dispersion relation is now

$$\omega^2 \rightarrow 2\lambda(1 - \cos k) + \Omega^2 \approx \lambda k^2 + \Omega^2. \quad (1.8)$$

The additional potential therefore creates a *gap* in the spectrum, so there are no solutions corresponding to any frequency below Ω .

To determine the normal modes we must impose boundary conditions. Suppose we take periodic boundary conditions by identifying atom $n + N$ with atom n . This means that η_n must equal η_{n+N} . Consequently, we require e^{ikN} to be unity and the allowed values of k are therefore

$$k_m = \frac{2\pi m}{N}, \quad m = 0, 1, \dots, N-1. \quad (1.9)$$

We can now write a normal-mode expansion

$$\eta_n(t) = \sum_{m=0}^{N-1} \{ A_m e^{ik_m n - i\omega_m t} + A_m^* e^{-ik_m n + i\omega_m t} \}. \quad (1.10)$$

Because the total displacement is a real number, we have added to each original complex exponential solution its complex conjugate.

From (1.1) we read off the momentum canonically conjugate to the displacement η_n

$$\pi_n \stackrel{\text{def}}{=} \frac{\partial L}{\partial \dot{\eta}_n} = \dot{\eta}_n. \quad (1.11)$$

In quantum mechanics the displacement η_n and its canonical conjugate π_n become operators $\hat{\eta}_n$ and $\hat{\pi}_n$ with commutation relations

$$[\hat{\eta}_n, \hat{\pi}_m] = i\hbar \delta_{nm}. \quad (1.12)$$

From (1.10) we find that

$$\pi_n(t) = \dot{\eta}_n(t) = \sum_{m=0}^{N-1} \{ -i\omega_m A_m e^{ik_m n - i\omega_m t} + i\omega_m A_m^* e^{-ik_m n + i\omega_m t} \}. \quad (1.13)$$

We have a choice as to how to include time evolution in the quantum mechanics formalism. In the Schrödinger¹ picture we put the time dependence in the Hilbert-space states and leave the operators time independent. This is the customary approach in elementary quantum mechanics courses, and is what we usually have in mind when we write equations like (1.12). In field theory it turns out to be more convenient to use the *Heisenberg*² picture where the operators are explicitly time dependent. For any operator \hat{O} we have

$$\hat{O}(t) = e^{\frac{i}{\hbar} \hat{H} t} \hat{O}(0) e^{-\frac{i}{\hbar} \hat{H} t}, \quad (1.14)$$

and

$$\frac{d\hat{O}}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{O}]. \quad (1.15)$$

When we use the Heisenberg picture, we must specify the times at which the fields in the commutation relation are to be evaluated. To retain its simple form (1.12) must be replaced by an equal-time commutator

$$[\hat{\eta}_n(t), \hat{\eta}_m(t)] = i\hbar \delta_{nm}. \quad (1.16)$$

Finding the commutator with the operators evaluated at two different times requires solving the dynamics of the system.

¹Erwin Schrödinger. Born August 12, 1887, Vienna. Died January 4, 1961, Vienna. Nobel Prize for Physics 1933.

²Werner Karl Heisenberg. Born December 5, 1901. Died February 1, 1976, Munich. Nobel Prize for Physics 1932.

1.1.2 Harmonic Oscillator

Let us recall how the Heisenberg picture works for the harmonic oscillator.

For a unit mass oscillator with angular frequency ω , the hamiltonian is

$$\hat{H} = \frac{1}{2}(\hat{p}^2 + \omega^2 \hat{x}^2). \quad (1.17)$$

Here the operators $\hat{x}(t)$ and $\hat{p}(t)$ obey the equal-time commutation relation

$$[\hat{x}(t), \hat{p}(t)] = i\hbar. \quad (1.18)$$

The equations of motion are

$$\frac{d\hat{x}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{x}] = \hat{p}(t), \quad (1.19)$$

$$\frac{d\hat{p}(t)}{dt} = \frac{i}{\hbar}[\hat{H}, \hat{p}] = -\omega^2 \hat{x}(t). \quad (1.20)$$

Differentiating the first equation with respect to t , and substituting for $\frac{d\hat{x}}{dt}$ from the second shows that

$$\frac{d^2 \hat{x}}{dt^2} + \omega^2 \hat{x} = 0. \quad (1.21)$$

The Heisenberg operator $\hat{x}(t)$ therefore satisfies exactly the same equation of motion as the classical variable $x(t)$ it replaces.

We could write down the solution to (1.21) in terms of sines and cosines, but it is more productive to introduce the operators $\hat{a}(t)$ and $\hat{a}^\dagger(t)$ by writing

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2\omega}}(\hat{a}(t) + \hat{a}^\dagger(t)) \quad (1.22)$$

$$\hat{p}(t) = \sqrt{\frac{\hbar}{2\omega}}(-i\omega\hat{a}(t) + i\omega\hat{a}^\dagger(t)). \quad (1.23)$$

Equivalently,

$$\hat{a}(t) = \sqrt{\frac{\omega}{2\hbar}}\left(\hat{x}(t) + i\frac{\hat{p}(t)}{\omega}\right), \quad (1.24)$$

$$\hat{a}^\dagger(t) = \sqrt{\frac{\omega}{2\hbar}}\left(\hat{x}(t) - i\frac{\hat{p}(t)}{\omega}\right). \quad (1.25)$$

Their equal-time commutation relations are found from those of \hat{x} , \hat{p} , to be

$$[\hat{a}(t), \hat{a}^\dagger(t)] = 1. \quad (1.26)$$

We also see that

$$\hat{H} = \hbar\omega(\hat{a}^\dagger(t)\hat{a}(t) + \frac{1}{2}). \quad (1.27)$$

So

$$\frac{d\hat{a}(t)}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{a}(t)] = -i\omega\hat{a}(t) \Rightarrow \hat{a}(t) = \hat{a}(0)e^{-i\omega t}, \quad (1.28)$$

$$\frac{d\hat{a}^\dagger(t)}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{a}^\dagger(t)] = +i\omega\hat{a}^\dagger(t) \Rightarrow \hat{a}^\dagger(t) = \hat{a}^\dagger(0)e^{+i\omega t}. \quad (1.29)$$

From now on we will write \hat{a} for $\hat{a}(0)$, and similarly for $\hat{a}^\dagger(0)$. In field theory these are called the *annihilation* and *creation* operators, respectively.

The time dependence of $\hat{x}(t)$ and $\hat{p}(t)$ is now explicit:

$$\hat{x}(t) = \sqrt{\frac{\hbar}{2\omega}} (\hat{a}e^{-i\omega t} + \hat{a}^\dagger e^{+i\omega t}), \quad (1.30)$$

$$\hat{p}(t) = \sqrt{\frac{\hbar}{2\omega}} (-i\omega\hat{a}e^{-i\omega t} + i\omega\hat{a}^\dagger e^{+i\omega t}). \quad (1.31)$$

If we substitute these expressions into the hamiltonian, we find that it is time independent

$$\hat{H} = \hbar\omega(\hat{a}^\dagger\hat{a} + \frac{1}{2}), \quad (1.32)$$

just as it is in classical mechanics.

1.1.3 Annihilation and Creation Operators for Normal Modes

Inspired by the harmonic oscillator, let us try setting

$$\hat{\eta}_n(t) = \sum_{m=0}^{N-1} \sqrt{\frac{\hbar}{2\omega_m}} \frac{1}{\sqrt{N}} \{ \hat{a}_m e^{ik_m n - i\omega_m t} + \hat{a}_m^\dagger e^{-ik_m n + i\omega_m t} \}, \quad (1.33)$$

$$\hat{\pi}_n(t) = \sum_{m=0}^{N-1} \sqrt{\frac{\hbar}{2\omega_m}} \frac{1}{\sqrt{N}} \{ -i\omega_m \hat{a}_m e^{ik_m n - i\omega_m t} + i\omega_m \hat{a}_m^\dagger e^{-ik_m n + i\omega_m t} \}, \quad (1.34)$$

where $[\hat{a}_m, \hat{a}_n^\dagger] = \delta_{mn}$, and computing the equal-time commutator, $[\hat{\eta}_n(t), \hat{\pi}_m(t)]$, to see if it comes out right. We have some hope that this will work since the $\sqrt{\frac{\hbar}{2\omega}}$'s are suggested by the harmonic-oscillator case, and the $\frac{1}{\sqrt{N}}$'s serve to normalize the normal modes.

In dealing with these sorts of sums it is useful to remember the finite Fourier series identity

$$\sum_{m=0}^{N-1} e^{ik_m(n-n')} = N\delta_{nn'}, \quad (1.35)$$

which is easily proved from the formula for the sum of a geometric progression.

A short calculation shows that everything works, and

$$[\hat{\eta}_n(t), \hat{\pi}_m(t)] = i\hbar\delta_{nm} \quad (1.36)$$

as it should.

We can also express the hamiltonian in terms of $\hat{a}_m, \hat{a}_m^\dagger$. We find

$$\hat{H} = \sum_n \left\{ \frac{1}{2} \hat{\pi}_n^2 + \frac{\lambda}{2} (\hat{\eta}_n - \hat{\eta}_{n+1})^2 \right\} = \sum_{m=0}^{N-1} \hbar\omega_m (\hat{a}_m^\dagger \hat{a}_m + \frac{1}{2}). \quad (1.37)$$

We now know essentially everything about our model crystal. We only need to remember how to construct the Hilbert space for the harmonic oscillator by acting with \hat{a}^\dagger on the ground state, and then generalize this to the crystal. Then we are home. Recall that in constructing the harmonic-oscillator operator representation we postulate the existence of a ground state $|0\rangle$ such that $\hat{a}|0\rangle = 0$, and then the states

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (1.38)$$

are normalized, $\langle n|n\rangle = 1$, energy eigenstates

$$\hat{H}|n\rangle = \hbar\omega(n + \frac{1}{2})|n\rangle. \quad (1.39)$$

Von Neumann³ proved that this representation of the harmonic oscillator operator algebra is unique.

The Hilbert space for the crystal is a tensor product of N copies of the harmonic oscillator space. This may sound complicated, but all we need is to assume that there is a state $|0\rangle$ that obeys

$$\hat{a}_m|0\rangle = 0, \quad \forall m. \quad (1.40)$$

Then

$$|n_0, n_1, \dots, n_{N-1}\rangle = \frac{(\hat{a}_0^\dagger)^{n_0}}{\sqrt{n_0!}} \frac{(\hat{a}_1^\dagger)^{n_1}}{\sqrt{n_1!}} \dots \frac{(\hat{a}_{N-1}^\dagger)^{n_{N-1}}}{\sqrt{n_{N-1}!}} |0\rangle \quad (1.41)$$

is a normalized eigenstate of

$$\hat{H} = \sum_{m=0}^{N-1} \hbar\omega_m (\hat{a}_m^\dagger \hat{a}_m + \frac{1}{2}), \quad (1.42)$$

with eigenvalue

$$E = E_0 + n_0\hbar\omega_0 + n_1\hbar\omega_1 + \dots + n_{N-1}\hbar\omega_{N-1}. \quad (1.43)$$

Here

$$E_0 = \sum \frac{1}{2} \hbar\omega_m. \quad (1.44)$$

³Johann (John) von Neumann. Born December 3, 1903, Budapest, Hungary. Died February 8, 1957, Washington DC.

The Hilbert space spanned by these states is called *Fock Space*.

We call the excited states *phonons*. We say that there are n_1 phonons in the first mode, n_2 in the second, and so on. They obey Bose statistics because the *occupation numbers* n_n may be as large as we wish. We think of the phonons as elementary “particles” that possess definite energy and momentum and may, when suitable interaction terms are included in the hamiltonian, scatter off one another just as any of the other “-ons” (mesons, photons, and so on) known to physics. The duality of the field [here $\hat{\eta}(x, t)$] and particle is the heart of quantum field theory.

1.2 Continuum Limit

1.2.1 Sums and Integrals

Now we stand back and blur our vision so that the atomic crystal appears as an elastic continuum. Viewed without a microscope the displacements η_n become a field $\eta(x)$, where x can be any real number. Naturally N must be taken very large so that we have some macroscopic size to our system.

Of course $x = na$ still, but we will be interested in slowly varying functions so that $f(an)$ can be regarded as a smooth function of x . The basic “rule” for this blurring is

$$a \sum_n f(an) \rightarrow \int f(an) a dn \rightarrow \int f(x) dx, \quad (1.45)$$

Now

$$a \sum_n f(na) \frac{1}{a} \delta_{nm} = f(ma) \rightarrow \int f(x) \delta(x - y) dx = f(y). \quad (1.46)$$

The Dirac delta function therefore corresponds to

$$\frac{\delta_{nn'}}{a} \rightarrow \delta(x - x'). \quad (1.47)$$

The divergent quantity $\delta(0)$ (in x space) is obtained by setting $n = n'$ and is thus to be understood as the reciprocal of the lattice spacing, or, equivalently, the number of normal modes per unit volume.

For Fourier sums we recall that

$$\sum_{m=0}^{N-1} e^{ik_m(n-n')} = N \delta_{nn'}, \quad (1.48)$$

where $k_m = \frac{2\pi m}{N}$. Since we want $k_m n = (k_m/a) na \rightarrow kx$, we must scale k so the continuum wavenumber is $k_m/a \rightarrow k$. In (1.48) the dimensionless k_m runs between 0 and 2π . We can equally well have the sum go symmetrically between $-\pi$ and $+\pi$, so the continuum k ranges between $-\frac{\pi}{a}$ and $+\frac{\pi}{a}$. Thus

$$\delta(x - x') \leftarrow \frac{\delta_{nn'}}{a} = \frac{1}{Na} \sum_m e^{ik_m(n-n')} \rightarrow \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(x-x')}. \quad (1.49)$$

The limits on the last integral should be $\pm \frac{\pi}{a}$, but, if we are only interested in functions varying slowly on the scale of a , we can take the limits on the integral to be infinite. This then is the usual Fourier-integral representation of the delta function.

It is good practice when doing Fourier transforms in field theory to treat x and k asymmetrically. Always put the 2π 's with the dk 's. This is because $\frac{dk}{2\pi}$ has the physical meaning of the number of normal modes per unit (spatial) volume with wavenumber between k and $k + dk$. In other words,

$$\sum_m F(k_m/a) = \sum_m F(k) \leftrightarrow Na \int \frac{dk}{2\pi} F(k) = (Volume) \int \frac{dk}{2\pi} F(k). \quad (1.50)$$

The Fourier integral for $\delta(k - k')$ is

$$\int dx e^{i(k-k')x} = 2\pi \delta(k - k'), \quad (1.51)$$

so $2\pi \delta(0)$ (in k space), although again mathematically divergent, has the physical meaning $\int dx = V$, the volume of the system. Again it is good practice to put a 2π with each $\delta(k)$, because this combination has a direct physical interpretation.

Note that the symbol $\delta(0)$ has a very different physical interpretation depending on whether δ is a delta function in x or in k space.

1.2.2 Continuum Fields

We might take the continuum version of our crystal lagrangian to be

$$L = T - V = \int dx \left\{ \frac{1}{2} \rho_0 \dot{\eta}(x)^2 - \frac{\kappa}{2} (\partial_x \eta)^2 \right\}, \quad (1.52)$$

where ρ_0 is the equilibrium mass density and $\eta(x)$ is the displacement field. The elastic constant κ is the one-dimensional equivalent of the bulk modulus. It is, however, common in field theory to absorb constants (in this case ρ_0) into the fields in order to make the coefficient of the kinetic term simply $\frac{1}{2}$. We can do this by defining $\varphi(x) = \sqrt{\rho_0} \eta(x)$. Then, after defining $\kappa/\rho_0 = c^2$, and adding a pinning term $\propto \varphi^2$, we will write

$$L = \int dx \left\{ \frac{1}{2} \dot{\varphi}^2 - \frac{c^2}{2} (\partial_x \varphi)^2 - \frac{m^2 c^4}{2} \varphi^2 \right\}. \quad (1.53)$$

The equation of motion can be found directly from the principle of least action. Here, as usual, the action S is defined by $S = \int dt L$. We can express the equation of motion as

$$\frac{\delta S}{\delta \varphi(x, t)} = 0, \quad (1.54)$$

where the functional (sometimes called the Fréchet) derivative $\delta/\delta \varphi$ is defined by

$$\delta S = \int dx dt \frac{\delta S}{\delta \varphi(x, t)} \delta \varphi(x, t). \quad (1.55)$$

In the present case we find, after integrating by parts and discarding the boundary terms, that

$$\delta S = \int dx dt (-\partial_t^2 \varphi + c^2 \partial_x^2 \varphi - m^2 c^4 \varphi) \delta \varphi, \quad (1.56)$$

so the equation of motion is

$$\partial_t^2 \varphi = c^2 \partial_x^2 \varphi - m^2 c^4 \varphi. \quad (1.57)$$

In the absence of the pinning term this is just the wave equation for wave speed c .

There are solutions

$$\varphi(x, t) = e^{ikx - i\omega_k t} \quad (1.58)$$

where ω_k is the positive square root of

$$\omega_k^2 = c^2 k^2 + m^2 c^4. \quad (1.59)$$

To quantize, we need the corresponding hamiltonian. We first define the canonically conjugate momentum field by

$$\pi(x) \equiv \frac{\delta L}{\delta \dot{\varphi}(x)} = \dot{\varphi}(x). \quad (1.60)$$

In evaluating this functional derivative, we regarded φ and $\dot{\varphi}$ as independent variables, as we always do in lagrangian mechanics. We then use the conjugate field to define the hamiltonian as $H = \sum p\dot{q} - L$, except that now we need to integrate, rather than sum, over the continuous variable x . We find

$$\begin{aligned} H &= \int dx (\pi(x) \dot{\varphi}(x) - L) \\ &= \int dx \left\{ \frac{1}{2} \dot{\varphi}^2 + \frac{c^2}{2} (\partial_x \varphi)^2 + \frac{m^2 c^4}{2} \varphi^2 \right\}. \end{aligned} \quad (1.61)$$

We now write down the quantum fields

$$\hat{\varphi}(x) = \int \frac{dk}{2\pi} \sqrt{\frac{\hbar}{2\omega_k}} \left\{ \hat{a}_k e^{+ikx - i\omega_k t} + \hat{a}_k^\dagger e^{-ikx + i\omega_k t} \right\} \quad (1.62)$$

and

$$\hat{\pi}(x) = \int \frac{dk}{2\pi} \sqrt{\frac{\hbar}{2\omega_k}} \left\{ -i\omega_k \hat{a}_k e^{+ikx - i\omega_k t} + i\omega_k \hat{a}_k^\dagger e^{-ikx + i\omega_k t} \right\}, \quad (1.63)$$

with

$$[\hat{a}_k, \hat{a}_{k'}^\dagger] = 2\pi \delta(k - k'). \quad (1.64)$$

Their equal-time commutator comes out to be

$$[\hat{\varphi}(x, t), \hat{\pi}(x', t)] = i\hbar \delta(x - x'). \quad (1.65)$$

This is exactly what is needed for the Heisenberg equations of motion to coincide with the classical ones.

The quantum hamiltonian \hat{H} can be written in terms of \hat{a}_k and \hat{a}_k^\dagger as

$$\hat{H} = \int \frac{dk}{2\pi} \frac{1}{2} \hbar \omega_k (\hat{a}_k^\dagger \hat{a}_k + \hat{a}_k \hat{a}_k^\dagger). \quad (1.66)$$

In writing this expression we have taken care to keep the $\hat{a}_k^\dagger, \hat{a}_k$'s in the ordering that they appear when we expand out the $\hat{\phi}$'s. If we use (1.55) and $Vol = 2\pi \delta(k=0)$, we see that

$$\hat{H} = E_0 + \int \frac{dk}{2\pi} \hbar \omega_k (\hat{a}_k^\dagger \hat{a}_k), \quad (1.67)$$

where the ground-state energy is

$$E_0 = (Vol) \int \frac{dk}{2\pi} \frac{1}{2} \hbar \omega_k = \sum_{modes} \frac{1}{2} \hbar \omega_k. \quad (1.68)$$

For a strictly continuous system there is no cut-off in the k integral and the zero point energy density is divergent. This is not necessarily a problem because this energy is only experimentally accessible when we have some control over either the ω_k or the density of states. We can, for example, obtain this control by confining the field in a resonant cavity whose size is variable. We may then measure *changes* in E_0 , which is then known as the *Casimir* energy. Another case where only changes in the energy are important occurs when one part of the system can modify the parameters of another part. Taking advantage of such coupling to lower the ground-state energy drives many examples of *spontaneous symmetry breaking*.

The divergence in the total zero-point energy *is* important when we consider quantum fields coupled to gravity. Any energy density acts a source for the gravitational field, and a uniform, divergent, vacuum energy density should give rise to a large cosmological constant. The smallness of the observed cosmological constant has prompted much theoretical speculation.

Of course everything we have done here can be extended to three dimensions. For a scalar field φ we have action

$$S = \int d^4x \mathcal{L}, \quad (1.69)$$

where

$$\mathcal{L} = \frac{1}{2} \dot{\varphi}^2 - \sum_{i=1}^3 \frac{c^2}{2} (\partial_i \varphi)^2 - \frac{m^2 c^4}{2} \varphi^2 \quad (1.70)$$

is the *lagrangian density*, and a mode expansion

$$\hat{\phi}(x) = \int \frac{d^3k}{(2\pi)^3} \sqrt{\frac{\hbar}{2\omega_k}} \left\{ \hat{a}_k e^{+i\mathbf{k}\cdot\mathbf{x} - i\omega_k t} + \hat{a}_k^\dagger e^{-i\mathbf{k}\cdot\mathbf{x} + i\omega_k t} \right\}, \quad (1.71)$$

with

$$[\hat{a}_k, \hat{a}_{k'}^\dagger] = (2\pi)^3 \delta^3(\mathbf{k} - \mathbf{k}'). \quad (1.72)$$

This gives

$$[\hat{\varphi}(\mathbf{x}, t), \partial_i \hat{\varphi}(\mathbf{x}', t)] = i\hbar \delta^3(\mathbf{x} - \mathbf{x}'), \quad (1.73)$$

and so on.