Classical theory of the harmonic crystal

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- Relation to the theory of elasticity
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Normal modes of a Bravais lattice

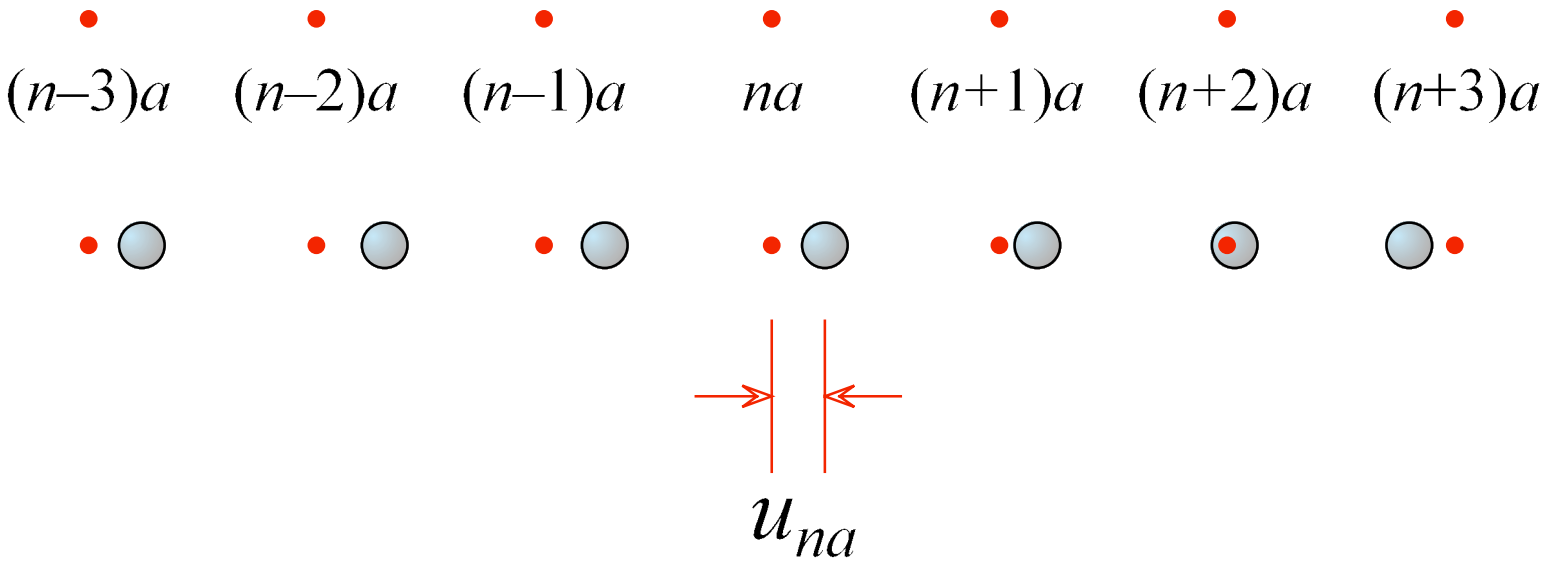
We will now examine the normal modes of a crystal lattice in the harmonic approximation.

The harmonic Hamiltonian is quadratic in the displacements and momenta. It represents a special case of the general classical problem of small oscillations that can be solved exactly.

The motion of N atoms can be represented as a linear combination of $3N$ normal vibrational modes, each with its own frequency. The set of frequencies of the $3N$ normal modes allows us, for example, construct all energy levels and to apply considerations of statistical mechanics.

We first discuss the normal modes of a one-dimensional monatomic Bravais lattice.

Consider a set of atoms of mass M that are equidistantly distributed along a line. Let the spacing of atoms in the chain be a. The vectors of the one-dimensional Bravais lattice are $\mathbf{R} = na$ with integer n.



Assume that the displacement of an atom is possible only along the line, and that only nearest neighbors interact. Let u_{na} be the displacement of the atom, which oscillates about na, from its equilibrium position.

The kinetic and potential energies of the atomic chain are

$$T = \frac{1}{2} M \sum_n \dot{u}_{na}^2$$

and

$$U = \frac{1}{2} K \sum_n \left[u_{na} - u_{(n+1)a} \right]^2 ,$$

respectively.

The force constant K can be expressed through the interaction energy $\phi(x)$ of two atoms separated by a distance x: $K = \phi''(a)$.

The Lagrangian is

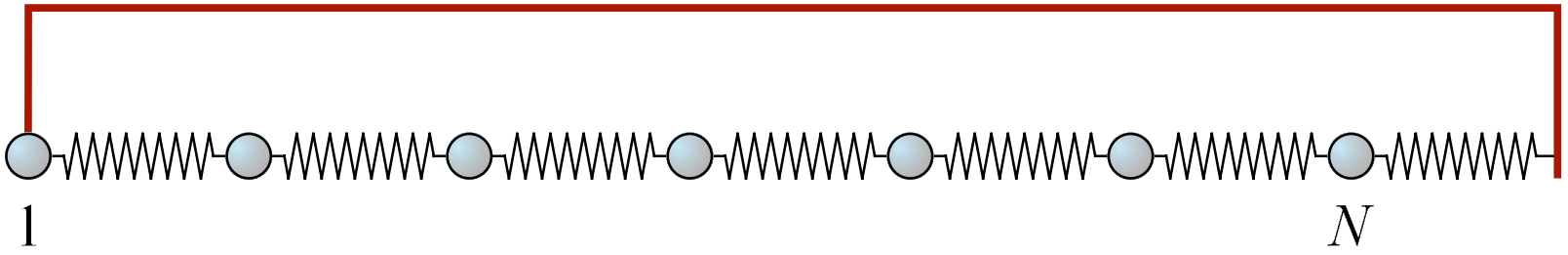
$$L = \frac{1}{2} M \sum_n \dot{u}_{na}^2 - \frac{1}{2} K \sum_n \left[u_{na} - u_{(n+1)a} \right]^2 \ .$$

The equations of motion are

$$M \ddot{u}_{na} = -K \left[2u_{na} - u_{(n-1)a} - u_{(n+1)a} \right] \ . \qquad (4.1)$$

Since the number N of atoms in the chain is large, the exact description of the atoms that are close to the ends of the chain is unimportant.

We therefore choose the Born-von Kármán periodic boundary condition. For a linear atomic chain this boundary condition can be formulated as follows: join the atom on the left end and the spring on the right end by a massless rigid rod of length $L = Na$.



Assume that the atoms occupy sites a, $2a$, $3a$, ..., Na.

Then we can use Eq. 4.1 to describe each of the N atoms $(n = 1, 2, ..., N)$.

The displacements $u_{(N+1)a}$ and u_0 that occur in the equations of motion for u_{Na} and u_a should replaced as follows:

$$u_{(N+1)a} = u_a\,; \quad u_0 = u_{Na}\ . \tag{4.2}$$

We seek solutions to (4.1) representing plane waves with angular frequency ω and wave vector k:

$$u_{na}(t) \sim e^{i(kna-\omega t)}\ . \tag{4.3}$$

We substitute (4.3) into the first of the conditions (4.2), cancel the common factor $e^{i(ka-\omega t)}$ and find that

$$e^{ikNa} = 1\ .$$

Therefore, k has the form:

$$k = \frac{2\pi}{a}\frac{j}{N} \ , \qquad (4.4)$$

where j is an integer.

Important: if k is changed by $2\pi/a$, the displacement u_a that is defined by (4.3) remains unchanged.

There are exactly N different solutions, corresponding to the N permitted values of the wave vector k consistent with (4.4).

We require these values to lie in the range between $-\pi/a$ and π/a.

We substitute (4.3) into (4.1) and find that

$$-M\omega^2 e^{i(kna-\omega t)} = -K\left(2 - e^{-ika} - e^{ika}\right)e^{i(kna-\omega t)} \quad . \qquad (4.5)$$

Cancelling the factor $e^{i(kna-\omega t)}$ and transforming the right-hand side of (4.5)

$$2 - e^{-ika} - e^{ika} = 2\left(1 - \operatorname{ch} ika\right) = 2\left(1 - \cos ka\right) = 4\sin^2\frac{ka}{2} \,,$$

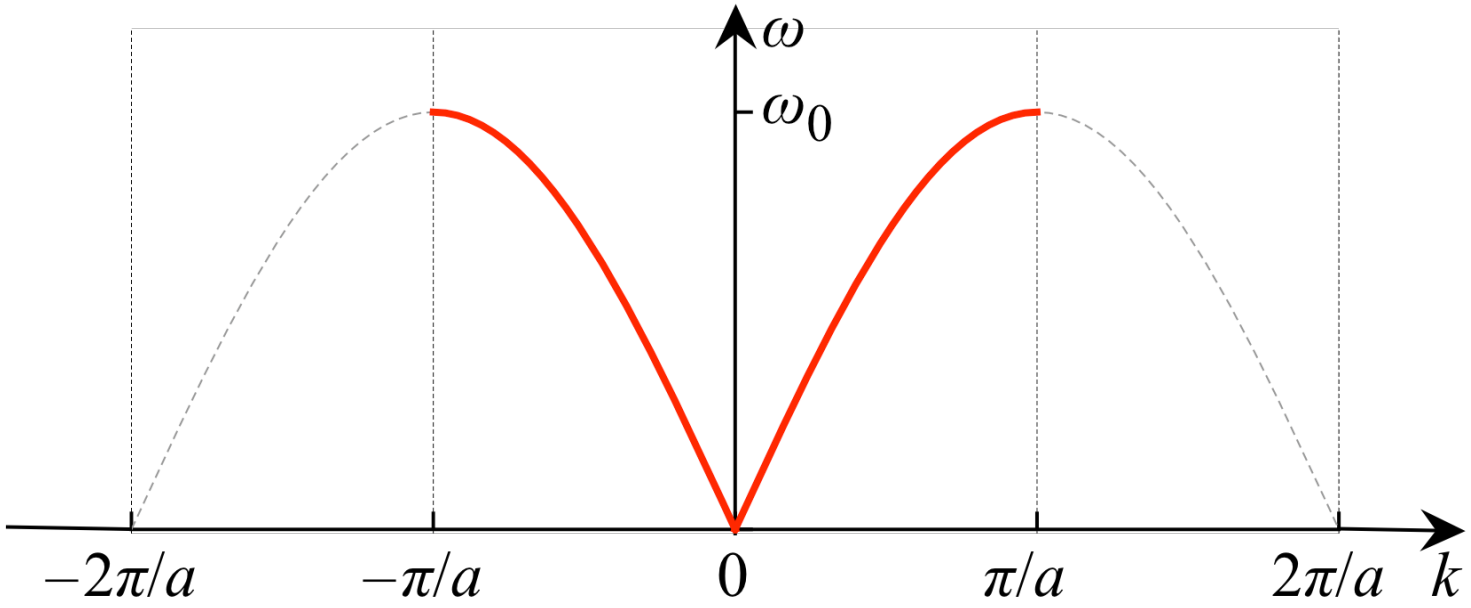
we find the characteristic equation

$$M\omega^2 = 4K\sin^2\frac{ka}{2} \,.$$

The equation of motion (4.1) has a solution for a given k if

$$\omega(k) = \omega_0 \left| \sin \frac{ka}{2} \right| , \qquad (4.6)$$

where $\omega_0 = 2\sqrt{K/M}$. Equation (4.6) is known as a dispersion curve.



The range of the wave vectors k between $-\pi/a$ and π/a is the first Brillouin zone of our one-dimensional lattice. The lattice parameter of the reciprocal lattice is $2\pi/a$.

The actual atomic displacements are given by the real or imaginary parts of (4.3):

$$u_{na}(t) \sim \cos(kna - \omega t), \qquad u_{na}(t) \sim \sin(kna - \omega t). \tag{4.7}$$

There are N different values of k, each with its own frequency $\omega(k)$, therefore (4.7) describes $2N$ independent solutions, which correspond to N normal modes.

Solutions (4.7) describe waves propagating along the linear chain of atoms. Their phase and group velocities are ω/k and $\partial\omega/\partial k$, respectively.

The group velocity

$$v_{\mathrm{G}} = \frac{\partial \omega}{\partial k} = \frac{\omega_0 a}{2} \cos \frac{ka}{2} \qquad (4.8)$$

decreases with increasing the wave vector k and vanishes at the Brillouin zone boundary π/a.

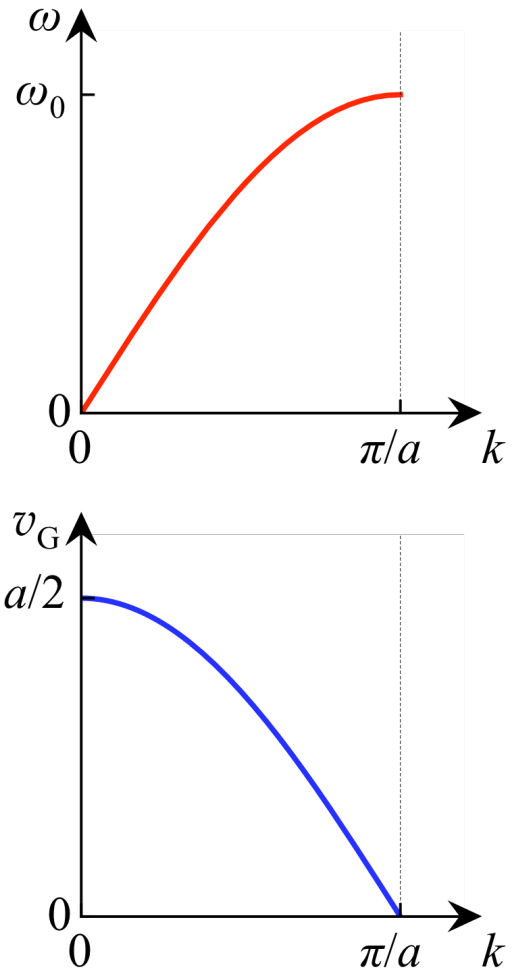


Fig. 75a

Waves with the wave vectors k that correspond to the Brillouin zone boundaries $k = \pm\pi/a$, are the standing waves

$$u_{na}(t) \sim e^{\pm in\pi} e^{-i\omega t} = u_0 (-1)^n e^{-i\omega t} \quad , \qquad (4.9)$$

in which the neighboring atoms move in opposition to one another.

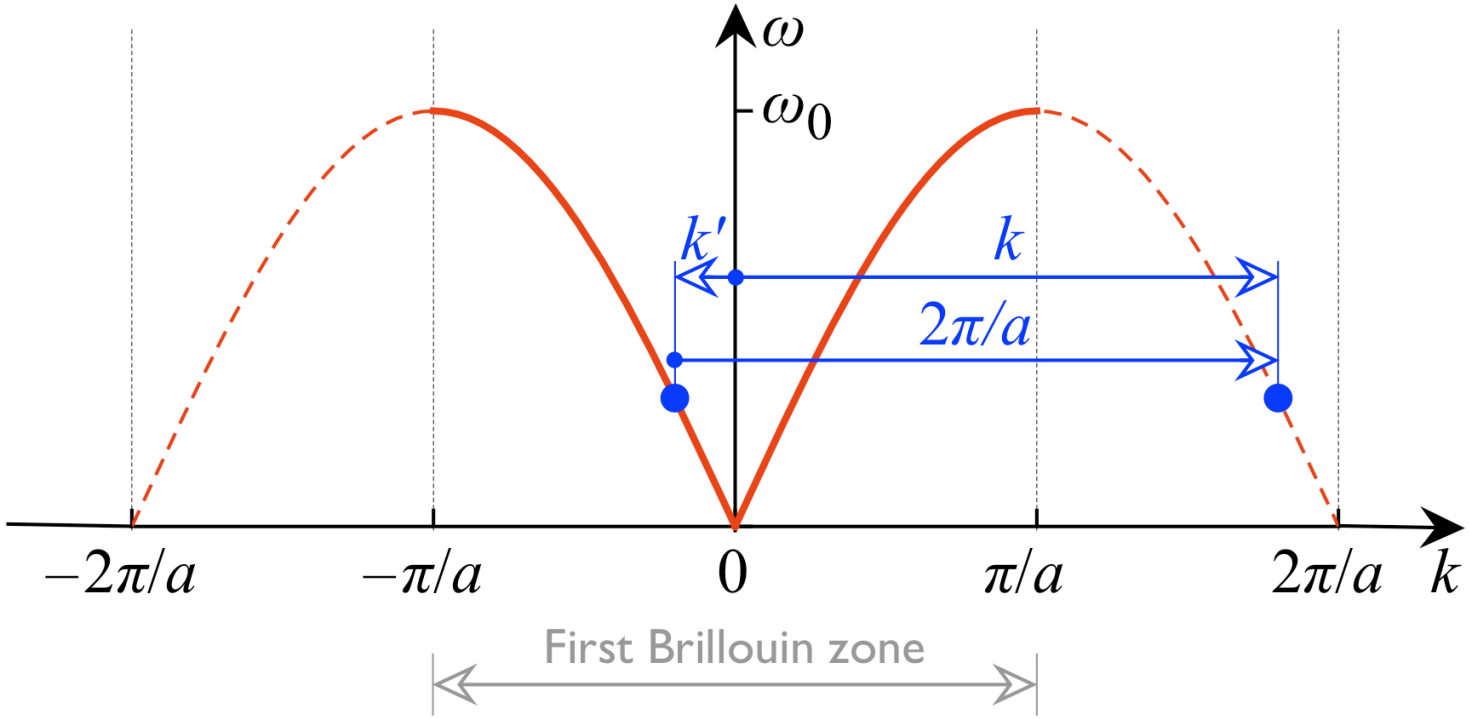
We note a close analogy of this phenomenon with the Bragg reflection of X-rays.

When the Bragg condition is satisfied, constructive interference of the incident and reflected waves results in a standing wave.

The wave vectors $k = \pm\pi/a$ that correspond to the boundaries of the first Brillouin zone satisfy the Bragg condition $2d\sin\theta = n\lambda$, if we take $\theta = \pi/2$, $d = a$, and the order of the reflection $n = 1$.

For $k = \pm\pi/a$ the wavelength $\lambda = 2a$, and the frequency ω reaches its maximum value of ω_0.

A solution with the wave vector k outside the first Brillouin zone is equivalent to the solution with the wave vector $k' = k - 2\pi j/a$, where j is integer, which is inside the first Brillouin zone. The two waves are indistinguishable if their wave vectors differ by the reciprocal lattice vector.



In the long wavelength $\lambda \gg a$ limit, where details of the structure do not play a significant role, the dispersion relation takes the form

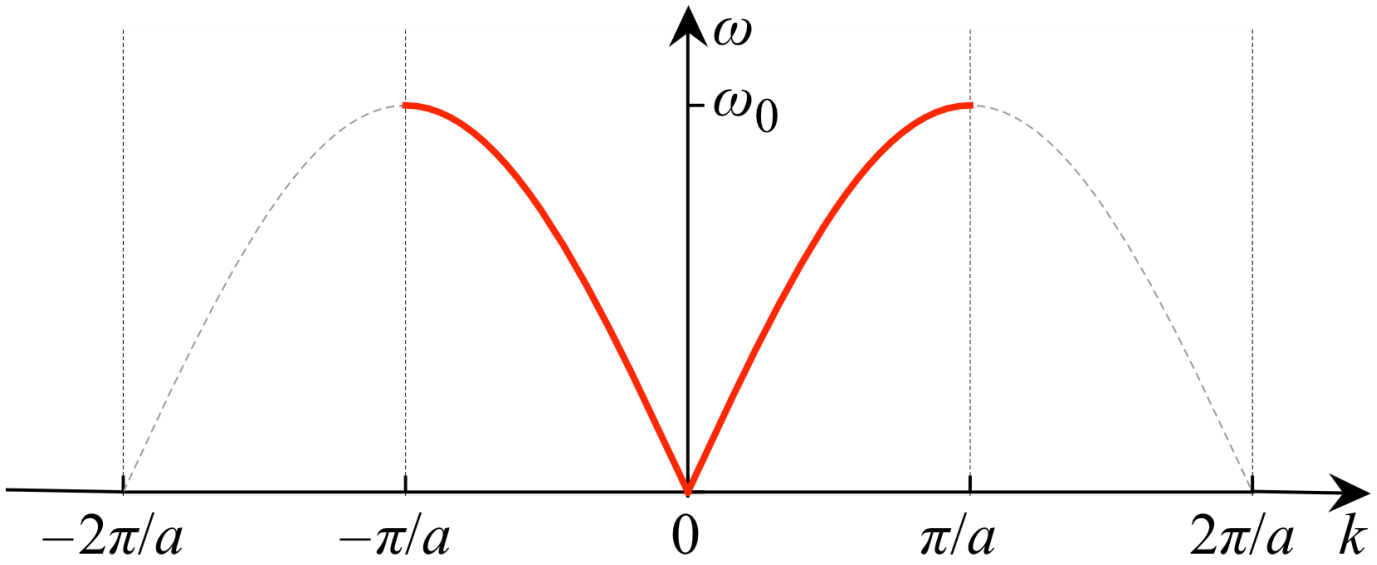
$$\omega = \frac{\omega_0 a}{2} k \ .$$

Since ω is linear in k, the group velocity is equal to the phase velocity and both are frequency independent.

Long-wavelength vibrations the chain can be looked at as vibrations of an elastic continuum.

Correspondingly, the long wavelength limit is the limit, in which the Debye model becomes applicable.

We now get back to the dispersion relation $\omega(k)$:



We attribute to a wave propagating in a one-dimensional monatomic lattice the frequency ω and the wave vector k, and, consequently, the 'momentum' $p = \hbar k$.

Such lattice waves can be thought of as having 'particle-like' properties. These 'particles' are known as phonons.

We now determine the density of normal modes.

The total number of normal modes is N, one mode per atom.

We remind that for a one-dimensional monatomic lattice with periodic boundary conditions a solution representing a propagating plane wave takes the form

$$u_{na}(t) \sim e^{i(kna-\omega t)} \quad .$$

The permitted wave vectors k are

$$k = \frac{2\pi}{a}\frac{j}{N} \quad ,$$

where j is an integer.

These wave vector values are equally spaced, and the separation between the neighboring values is $\Delta k = 2\pi/Na$.

The number of normal modes per unit wave vector is $Na/2\pi$ for k in the range $-\pi/a \le k \le \pi/a$ and zero for all other values of k.

We now define the density of normal modes $g(\omega)$. The number of normal modes $g(\omega)d\omega$ in the infinitesimal frequency range between ω and $\omega + d\omega$ is

$$g(\omega)d\omega = \frac{Na}{\pi}\frac{1}{\dfrac{\partial\omega}{\partial k}}d\omega \ . \qquad (4.10)$$

The group velocity $\partial\omega/\partial k$ can be determined from the dispersion relation $\omega(k)$.

The density of normal modes $g(\omega)$ has singularities when the group velocity vanishes, i.e., when the dispersion curve $\omega(k)$ becomes flat.

Expressing the wave vector k as a function of ω

$$k = \frac{2}{a} \arcsin \frac{\omega}{\omega_0} \ .$$

we have

$$\frac{dk}{d\omega} = \frac{2}{a} \frac{1}{\sqrt{\omega_0^2 - \omega^2}} \ . \qquad (4.11)$$

If we substitute (4.11) into (4.10), we find that

$$g(\omega) = \frac{2N}{\pi} \frac{1}{\sqrt{\omega_0^2 - \omega^2}} \quad . \tag{4.12}$$

The density of normal modes $g(\omega)$ diverges as the frequency ω approaches ω_0.