The vibrations of one dimensional monoatomic lattice

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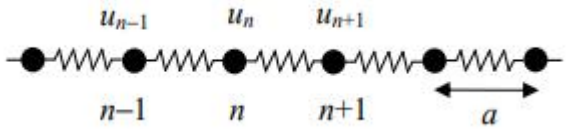
- One-dimensional lattice For simplicity we consider, first, a one-dimensional crystal lattice and assume that the forces between the atoms in this lattice are proportional to relative displacements from the equilibrium positions.



This is known as the harmonic approximation, which holds well provided that the displacements are small. One might think about the atoms in the lattice as interconnected by elastic springs. Therefore, the force exerted on n-the atom in the lattice is given by

$$F_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n),$$

- where C is the interatomic force (elastic) constant. Applying Newton's second law to the motion of the n-th atom we obtain

$$M\frac{d^2u_n}{dt^2} = F_n = C(u_{n+1} - u_n) + C(u_{n-1} - u_n) = -C(2u_n - u_{n+1} - u_{n-1}),$$

- where M is the mass of the atom. Note that we neglected here by the interaction of the n-th atom with all but its nearest neighbors. A similar equation should be written for each atom in the lattice, resulting in N coupled differential equations, which should be solved simultaneously (N is the total number of atoms in the lattice). In addition the boundary conditions applied to the end atom in the lattice should be taken into account. Now let us attempt a solution of the form

$$u_n = Ae^{i(qx_n - \omega t)}$$

- where xn is the equilibrium position of the n-th atom so that xn=na. This equation represents a traveling wave, in which all the atoms oscillate with the same frequency ω and the same amplitude A and have wavevector q. Note that a solution of the form (5.3) is only possible because of the transnational symmetry of the lattice. Now substituting Eq.(5.3) into Eq.(5.2) and canceling the common quantities (the amplitude and the time-dependent factor) we obtain

$$M(-\omega^2)e^{iqna} = -C\left[2e^{iqna} - e^{iq(n+1)a} - e^{iq(n-1)a}\right]$$

- This equation can be further simplified by canceling the common factor iqna e , which leads to

$$M\omega^2 = C\left(2 - e^{iqa} - e^{-iqa}\right) = 2C\left(1 - \cos qa\right) = 4C\sin^2\frac{qa}{2}.$$

- We find therefore the dispersion relation for the frequency

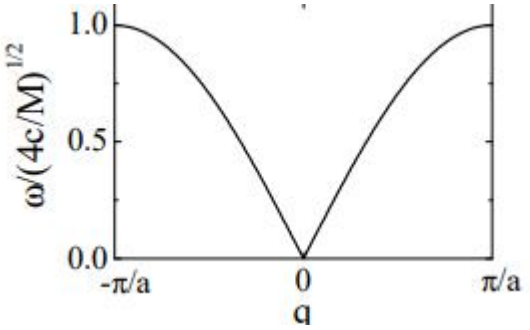
- which is the relationship between the frequency of vibrations and the wavevector q. This dispersion relation have a number of important properties.

$$\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{qa}{2}\right|,$$

- (i) Reducing to the first Brillouin zone. The frequency (5.6) and the displacement of the atoms (5.3) do not change when we change q by q+2π/a. This means that these solutions are physically identical. This allows us to set the range of independent values of q within the first Brillouin zone, i.e.

$$-\frac{\pi}{a} \le q \le \frac{\pi}{a}.$$

- Within this range of q the ω versus q is shown in Fig.2.



- The maximum frequency is 4C / M . The frequency is symmetric with respect to the sign change in q, i.e. ω(q)= ω(-q). This is not surprising because a mode with positive q corresponds to the wave traveling in the lattice from the left to the right and a mode with a negative q corresponds to the wave traveling from the right tot the left. Since these two directions are equivalent in the lattice the frequency does not change with the sign change in q. At the boundaries of the Brillouin zone q=±π/a the solution represents a standing wave (1) n i $u_n = A(-1)^n e^{-i\omega t}$: – : atoms oscillate in the opposite phases depending on whether n is even or odd. The wave moves neither right nor left. (ii) Phase and group velocity. The phase velocity is defined by

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- and the group velocity by

$$v_g = \frac{d\omega}{dq}.$$

- The physical distinction between the two velocities is that vp is the velocity of the propagation of the plane wave, whereas the vg is the velocity of the propagation of the wave packet. The latter is the velocity for the propagation of energy in the medium. For the particular dispersion relation (5.6) the group velocity is given by

$$v_g = \sqrt{\frac{Ca^2}{M}} \cos\frac{qa}{2}.$$

- As is seen from Eq.(5.10) the group velocity is zero at the edge of the zone where q=±π/a. Here the wave is standing and therefore the transmission velocity for the energy is zero. (iii) Long wavelength limit. The long wavelength limit implies that λ>>a. In this limit qa<

$$\omega = \sqrt{\frac{C}{M}} qa \, .$$

- We see that the frequency of vibration is proportional to the wavevector. This is equivalent to the statement that velocity is independent of frequency. In this case

$$v_p = \frac{\omega}{q} = \sqrt{\frac{C}{M}} a \, .$$

- This is the velocity of sound for the one dimensional lattice which is consistent with the expression we obtained earlier for elastic waves.