Physics with neutrons 1

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Exercise sheet 11
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Exercise 11.1

Derive the intermediate scattering function, pair correlation function, and the scattering law $S(\mathbf{Q},\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t} I(\mathbf{Q},t)$ for a single atom that oscillates harmonically in one dimension with a frequency ω_0. When you perform the Fourier transform, assume that the amplitude of the oscillation is very small.

Solution. We start with the intermediate scattering function in one dimension:

$$I(Q,t) = \frac{1}{N}\sum_{j,j'}\langle e^{-iQr_{j'}(0)} e^{iQr_j(t)}\rangle$$

For a single atom, we have $N = 1$ and therefore

$$I(Q,t) = \langle e^{-iQr_j(0)} e^{iQr_j(t)}\rangle = \langle e^{-iQ(r_j(0)-r_j(t))}\rangle.$$

Set $\rho(t) = r(t) - r(0)$. For a harmonic oscillation $\rho(t) = \rho_0\cos(\omega_0 t)$. Since the cosine is an even function, $r(t) - r(0) = r(0) - r(t)$. This gives us

$$I(Q,t) = \langle e^{-iQ\rho_0\cos(\omega_0 t)}\rangle$$

As given in the exercise, the amplitude ρ_0 is very small, so we can Taylor-expand the exponential:

$$I(Q,t) = \langle 1 - iQ\rho_0\cos(\omega_0 t) - \frac{1}{2}Q^2\rho_0^2\cos^2(\omega_0 t) + \frac{i}{6}Q^3\rho_0^3\cos^3(\omega_0 t) \pm ...\rangle.$$

All terms with odd powsers of the cosine vanish and therefore we are left with

$$I(Q,t) = 1 - \frac{1}{6}Q^2\rho_0^2, \qquad \text{using } \langle\cos^2 x\rangle = \frac{1}{3}.$$

Taking all terms into account, we arrive at

$$I(Q,t) = e^{-\frac{1}{6}Q^2\rho_0^2}$$

(which is analogous to the derviation of the Debye-Waller factor).
The pair correlation function is

$$G(r,t) = \frac{1}{2\pi}\int dQ\, e^{-iQr} I(Q,t) = \frac{1}{2\pi}\int dQ\, e^{-iQr} e^{-\frac{1}{6}Q^2\rho_0^2} = \sqrt{\frac{3}{2\pi}}\frac{1}{\rho_0}\exp\left(-\frac{3r^2}{2\rho_0^2}\right).$$

The scattering law is

$$S(Q,\omega) = \frac{1}{2\pi\hbar}\int dt\, e^{-i\omega t} I(Q,t) = \frac{1}{2\pi\hbar}\int dQ\, e^{-i\omega t} e^{-\frac{1}{6}Q^2\rho_0^2} = \exp\left(-\frac{1}{6}Q^2\rho_0^2\right)\delta(\hbar\omega).$$

Exercise 11.2

Prove that from the knowledge of the dispersion relation ω_q it is possible to determine the force constants k_n using the relation

$$k_n = -\frac{Ma}{2\pi}\int_{-\pi/a}^{\pi/a} \omega_q^2 \cos(nqa)dq.$$

Solution. From the dispersion relation we have

$$\frac{M}{2}\omega^2 = \sum_n k_n(1-\cos(n\cdot qa)).$$

We multiply both sides with $\cos(m\cdot ka)$ and perform an integration over the interval $[-\pi/a, \pi/a]$

$$\int_{-\pi/a}^{\pi/a} dq\,\frac{M}{2}\omega^2\cos(m\cdot qa) = \int_{-\pi/a}^{\pi/a} dq\sum_n k_n(1-\cos(n\cdot qa))\cos(m\cdot qa) = -\frac{2\pi}{a}k_m.$$

The last relation holds, since

$$\frac{a}{2\pi}\int_{-\pi/a}^{\pi/a} dq\,\cos(m\cdot qa)\cos(n\cdot qa) = \delta_{mn}.$$

Rearranging the terms, we get

$$k_m = \frac{Ma}{2\pi}\int_{-\pi/a}^{\pi/a} dk\,\omega^2\cos(m\cdot qa)$$

□

Exercise 11.3

The acoustic phonon branches of many "simple" compounds are well explained by the sinusoidal dispersion relation derived in the lecture. The transverse acoustic phonon branches observed for germanium, however, exhibit an unusual flattening of the dispersion relation upon approaching the zone boundary (Fig. 2). Germanium is a semiconductor with covalent bonds which are usually formed from two electrons, one from each atom participating in the bond. These electrons tend to be partially localized midway between the two atoms and constitute the so-called bond charge (Fig. 1). Derive the phonon dispersion for the one-dimensional chain illustrated in Fig. 1 by following the procedure for a diatomic one-dimensional chain from the lecture.

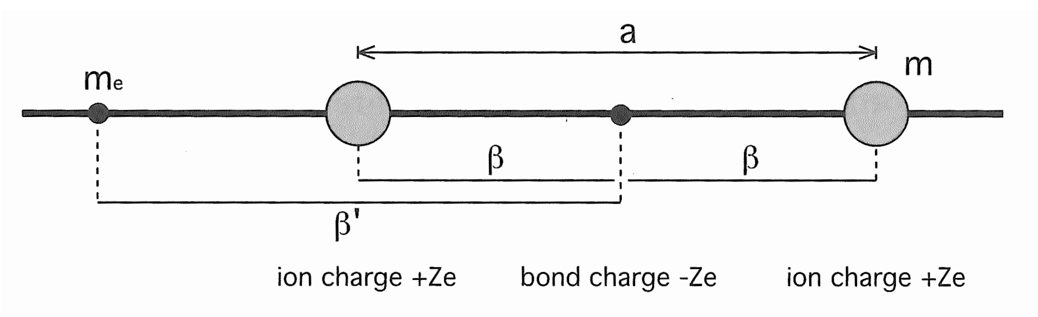

Figure 1: Linear chain formed by alternating ion and bond charges. Bond charges are connected via effective force constants β and β' to neighboring ion and bond charges, respectively.

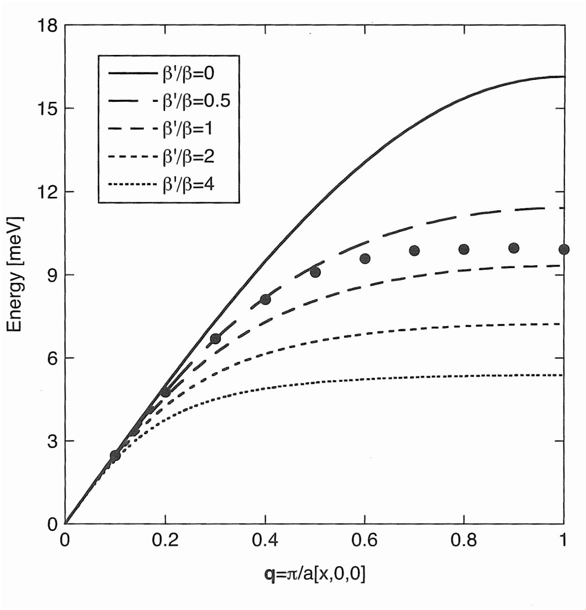

Figure 2: Dispersion relation of the lower transverse acoustic phonon branch measured for Ge at 80 K along the [100] direction (after [Nellin and Nilsson (1972)]).

Solution. As sketched in Fig. 1, we denote the force constant between an atom of mass m and the bond charge of mass m_e by β. In addition, we introduce the force constant β' to describe the interaction between two bond charges. In analogy to the diatomic one-dimensional chain, we get for the equations of motion

$$m\ddot{u}_{2n} = \beta(u_{2n+1} + u_{2n-1} - 2u_{2n}), \tag{1}$$

$$m_e\ddot{u}_{2n+1} = \beta(u_{2n+2} + u_{2n} - 2u_{2n+1} + \beta'(u_{2n+3} + u_{2n-1} - 2u_{2n+1}) = 0, \tag{2}$$

where we set $m_e = 0$ since $m_e \ll m$. Inserting the ansatz

$$u2n = \xi e^{i(\omega t + 2nqa)}, \qquad u2n + 1 = \eta e^{i(\omega t + 2nqa)}$$

into the Eqs. (1) and (2) we get

$$m\omega^2\eta = 2\beta\left(\eta - \xi\cos\left(\frac{qa}{2}\right)\right),$$

$$\beta\left(\eta\cos\left(\frac{qa}{2}\right) - \xi\right) + \beta'\xi(\cos(qa) - 1) = 0,$$

from which we obtain a relation between the amplitudes ξ and η:

$$\xi = \frac{\beta\cos(qa/2)}{\beta + 2\beta'\sin^2(qa/2)}.$$

Substituting this into Eq. (1) yields [Brüesch (1982)]

$$\omega(q) = \sqrt{\frac{1}{m}\cdot\frac{2\beta(\beta + 2\beta')\sin^2(qa/2)}{\beta + 2\beta'\sin^2(qa/2)}}. \tag{3}$$

For $q \ll \pi/a$ we get the limit

$$\omega(q) = \sqrt{\frac{\beta + 2\beta'}{2m}}qa = \sqrt{\frac{c}{\rho}}q = vq,$$

where we use the same notation as for the linear chain with two different atoms. Fig. 2 shows dispersion curves calculated from Eq. (3) for different ratios β'/β. We see that the acoustic phonon branch of Ge can be modelled with the ration $0.5 < \beta'/\beta < 1$. □