LMU München
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Lehrstuhl für Theoretische Nanophysik
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5. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Thursday, November 24, 2016.

Exercise 1: Normal modes of a three-dimensional crystal

Consider a face-centered cubic monoatomic Bravais lattice in which each ion interacts only with its twelve nearest neighbours. Assume that the interacion between a pair of neighbouring ions is described by a pair potential ϕ that depends only on the distance r between the pair of ions.

a. Show that the frequencies of the three normal modes with a wave vector $\boldsymbol{k}$ are given by $\omega = \sqrt{\lambda/M}$, where the λ are the eigenvalues of the 3×3 matrix,

$$\boldsymbol{D} = \sum_{\boldsymbol{R}} \sin^2(\boldsymbol{k} \cdot \boldsymbol{R}/2) \left[A\mathbf{1} + B\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}\right]. \tag{1}$$

Here the sum is over the twelve nearest neighbours of $\boldsymbol{R} = 0$: $\left\{\frac{a}{2}(\pm\hat{x} \pm \hat{y}), \frac{a}{2}(\pm\hat{y} \pm \hat{z}), \frac{a}{2}(\pm\hat{x} \pm \hat{z})\right\}$. $\mathbf{1}$ is the unit matrix ($[\mathbf{1}]_{\mu,\nu} = \delta_{\mu,\nu}$) and $\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}$ is the diadic form of the unit vectors $\hat{\boldsymbol{R}} = \boldsymbol{R}/R$ (i.e. $[\hat{\boldsymbol{R}}\hat{\boldsymbol{R}}]_{\mu,\nu} = \hat{\boldsymbol{R}}_\mu \hat{\boldsymbol{R}}_\nu$). The constants A and B are given by $A = 2\phi'(d)/d$ and $B = 2[\phi''(d) - \phi'(d)/d]$, where d is the equilibrium nearest-neighbour distance.

b. Show that when $\boldsymbol{k}$ is along the $[1, 0, 0]$ direction (i.e. $\boldsymbol{k} = (k, 0, 0)$), one normal mode is strictly longitudinal, with frequency

$$\omega_L = \sqrt{\frac{8A + 4B}{M}} \sin(|k|a/4) \ ,$$

and the other two are strictly transverse and degenerate, with frequency

$$\omega_T = \sqrt{\frac{8A + 2B}{M}} \sin(|k|a/4) \ .$$

c. What are the frequencies and polarizations of the normal modes when $\boldsymbol{k}$ is along the $[1, 1, 1]$ direction (i.e. take $\boldsymbol{k} = (k, k, k)/\sqrt{3}$) ?

d. Show that when $\boldsymbol{k}$ is along the [110] direction (i.e. $\boldsymbol{k} = (k, k, 0)/\sqrt{2}$), then one mode is strictly longitudinal, with frequency

$$\omega_L = \sqrt{\frac{8A + 2B}{M} \sin^2\left(\frac{ka}{4\sqrt{2}}\right) + \frac{2A + 2B}{M} \sin^2\left(\frac{ka}{2\sqrt{2}}\right)},$$

one is strictly transverse and polarized along the z-axis with frequency

$$\omega_T^{(1)} = \sqrt{\frac{8A+4B}{M}\sin^2\left(\frac{ka}{4\sqrt{2}}\right) + \frac{2A}{M}\sin^2\left(\frac{ka}{2\sqrt{2}}\right)},$$

and the third is strictly transverse and perpendicular to the z-axis, with frequency

$$\omega_T^{(2)} = \sqrt{\frac{8A+2B}{M}\sin^2\left(\frac{ka}{4\sqrt{2}}\right) + \frac{2A}{M}\sin^2\left(\frac{ka}{2\sqrt{2}}\right)}.$$

Exercise 2: Diatomic chain

Consider a linear chain in which ions on alternating positions have mass M_1 and M_2. Treat the system in harmonic approximation for nearest neighbor interactions with spring constant K.

a. Show that the dispersion relation for the normal phonon modes is

$$\omega^2 = \frac{K}{M_1 M_2}(M_1 + M_2 \pm \sqrt{M_1^2 + M_2^2 + 2M_1 M_2 \cos(ka)}). \tag{2}$$

b. Discuss the form of the dispersion relation and the nature of the normal modes when $M_1 \gg M_2$.

c. Compare the dispersion relation (2) with that of a monatomic chain,

$$\omega_{mon}(k) = 2\sqrt{\frac{K}{M}}\left|\sin(\frac{1}{2}ka)\right|,$$

when $M_1 \approx M_2$.