Solid State Theory

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Exercise 1: Harmonic approximation for a classical N-particle system

In Sec. 3.1 'The harmonic approximation', a diagonal form of the ionic Hamiltonian

$$H_{\text{harm}} = \sum_{j=1}^{Nd} \hbar\omega_j \left(b_j^\dagger b_j + \tfrac{1}{2} \right) \;, \qquad (1)$$

has been derived with the approximation that the effective potential $V_{\text{eff}}(\vec{R})$ is expanded up to second order in the displacements. The squares of the ω_j appearing in eq. (1) are given by the eigenvalues of the dynamical matrix D. Consider the corresponding classical system: a lattice of weights (with mass m) connected by springs (with spring constant k). Show that the frequencies ω_j of the eigenmodes follow from the diagonalization of precisely the same matrix D. (5 points)

Exercise 2: Lattice vibrations on a square lattice

Consider a two-dimensional square lattice with lattice spacing a. The lattice vectors $\vec{R}_n$ of this Bravais lattice correspond to the equilibrium positions of ions with mass M. The harmonic approximation of the effective potential in the ionic Hamiltonian is of the form

$$V = \frac{\alpha}{2} \sum_{\vec{n}} \left[\Big(\vec{u}(\vec{R}_{\vec{n}} + \vec{a}_1) - \vec{u}(\vec{R}_{\vec{n}}) \Big)^2 + \Big(\vec{u}(\vec{R}_{\vec{n}} + \vec{a}_2) - \vec{u}(\vec{R}_{\vec{n}}) \Big)^2 \right]$$

with

$$\vec{a}_1 = \begin{pmatrix} a \\ 0 \end{pmatrix} \;,\; \vec{a}_2 = \begin{pmatrix} 0 \\ a \end{pmatrix} \;,$$

and $\vec{u}(\vec{R}_{\vec{m}})$ the displacement of the ion with equilibrium position $\vec{R}_{\vec{m}}$.

Calculate the dispersion relation $\omega(\vec{q})$ of this system. (7 points)

Exercise 3: Linear chain with a basis of two ions

Consider a one-dimensional lattice with lattice spacing $2a$. The equilibrium positions of the ions with mass m_μ ($\mu = 1, 2$) are given by

$$R_{n,\mu} = R_n + R_\mu \ ,$$

with $R_n = 2na$, $R_{\mu=1} = 0$, and $R_{\mu=2} = a$. The two ions of the basis have different masses, $m_1 = m$ and $m_2 = M$. The effective potential for this system corresponds to that of a classical harmonic chain with springs between neighbouring ions (spring constant k).

a) Show that the dispersion relation of this system is given by

$$\omega^2 = \frac{k}{Mm} \left[M + m \pm \sqrt{M^2 + m^2 + 2Mm\cos(2qa)} \right]$$

(4 points)

b) Consider the limits $qa \to 0$ and $qa \to \pi/2$ and give a rough sketch of $\omega(q)$. (2 points)

c) Show that for $m = M$, the dispersion relation reduces to that of a mono-atomic chain. (2 points)