University of Regensburg | Summer Term 2018

Quantum Theory of Condensed Matter I

Prof. John Schliemann
Dr. Paul Wenk

Mo. 08:00-10:00 c.t., PHY 5.0.21

Sheet 2

1. Diatomic Chain .... [8P]

We are going to analyze vibrations of compound lattices. Let us consider the chain shown in Fig. 1. One can see that the elementary cell contains two atoms of mass M_1 and M_2. We make the approximation that the interaction between the atoms is only between nearest neighbors and that the force is quasi elastic with two different spring constants C_1, C_2 as depicted in Fig. 1.

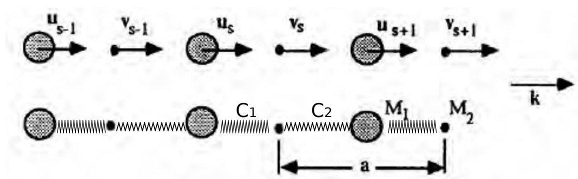

Figure 1: Diatomic Chain

(a)(2P) Determine the primitive translations and the vectors of the lattice and the reciprocal lattice. What is here the first Brillouin-Zone?

(b)(2P) Write down the equations of motion for the longitudinal lattice vibrations and solve them by using the ansatz $u_n = A_u e^{i(qan-\omega t)}$, $v_n = A_v e^{i(qan-\omega t)}$, where q is the wave vector, n the site index and ω the frequency. Why is this ansatz reasonable?

(c)(2P) Sketch the possible vibration branches and analyze the following cases:

1. $q = 0$,
2. $q = \pm\pi/a$,
3. $0 < q \ll \pi/a$.

(d)(2P) What happens to the modes in the degenerate case, i.e. when $C_1 = C_2$, $M_1 = M_2$?

2. Dynamical Matrix .... [7P]

Assume a *simple cubic lattice* with a lattice constant a. To describe the lattice vibrations we apply, as in Ex.1, the harmonic approximation including, however, both nearest neighbors (nn), which are coupled through the spring constant C_1, and next nearest neighbors (nnn), which are coupled through the spring constant C_2. Thus, the according potential V is given by

$$V = \frac{1}{2}\sum_{\mathbf{R}}\left(\frac{C_1}{2a^2}\sum_{\boldsymbol{D}\mathrm{nn}}(\mathbf{D}\cdot(\mathbf{u}_{\mathbf{R}+\mathbf{D}}-\mathbf{u}_{\mathbf{R}}))^2 + \frac{C_2}{4a^2}\sum_{\mathbf{D}'\mathrm{nnn}}(\mathbf{D}'\cdot(\mathbf{u}_{\mathbf{R}+\mathbf{D}'}-\mathbf{u}_{\mathbf{R}}))^2\right), \tag{1}$$

with the vectors $\mathbf{D}$ connecting the nn (these are $(\pm a,0,0)$, $(0,\pm a,0)$, $(0,0,\pm a)$) and $\mathbf{D}'$ connecting the nnn and the small elongations $\mathbf{u}$ at the position $\mathbf{R}$. The lattice vector $\mathbf{R}$ can be represented via triplets of integers (n,m,l). In case of a phonon with a wave vector $\mathbf{k} = k(1,0,0)$ in the reciprocal space the dynamical matrix $\mathbf{\Lambda}$ is diagonal. Calculate the phonon dispersion for this special direction.

Hint: Use proper indexing as $\mathbf{D}\cdot(\mathbf{u}_{\mathbf{R}+\mathbf{D}}-\mathbf{u}_{\mathbf{R}}) = a(u^x_{n\pm1,m,l}-u^x_{n,m,l})$ for $\mathbf{D} = \pm a\mathbf{e}_x$. Apply the eigenfunctions of the translation operator, $u^x_{nml} = A^x_{\mathbf{k}}\exp[i(nk_x + mk_y + lk_z)a]$, (for y,z respectively), to get an algebraic equation. Use the symmetry of the lattice.