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Problems for *Physik der Materie III*

Due by May 15, 2019

Series 4: Brillouin Zone and Phonons

4.1 Brillouin zone

The first Brillouin zone is defined as the Wigner-Seitz primitive cell of the reciprocal lattice. The n^{th} Brillouin Zone can be defined as the region of k-space that can be reached from the origin at Γ by crossing exactly $n-1$ Bragg planes. Bragg planes bisect the lines joining the origin to neighboring points of the reciprocal lattice.

(1) Sketch the first three Brillouin zones of the two-dimensional square lattice. Indicate the different zones and the Bragg "planes".

(2) Briefly explain the physical significance of the first Brillouin zone in relation to the phonon dispersion in crystals.

4.2 Graphene

Graphene is a two-dimensional (2d) crystal consisting of carbon atoms ordered in a lattice as indicated in Fig. 1. The vectors $\vec{r}_1$, $\vec{r}_2$ and $\vec{r}_3$ connect neighboring carbon atoms and make angles of 120° with each other. We assume that $\vec{r}_1$ is pointing in the direction of the positive x axis. The nearest neighbor distance is d.

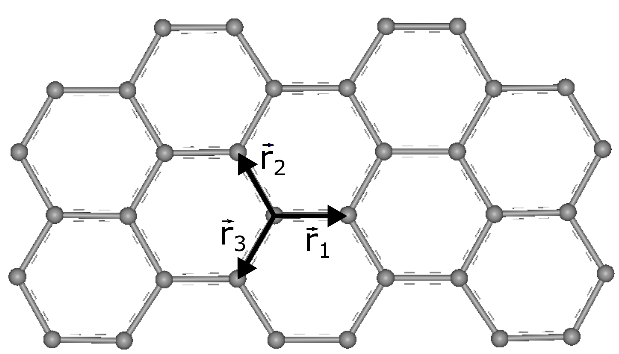

Figure 1: Graphene structure

(1) Sketch a primitive unit cell. How many carbon atoms does it contain? Give a vector expression for the primitive lattice vectors $\vec{a}_1$ and $\vec{a}_2$, and draw them in your sketch.

(2) Construct the 2d reciprocal lattice of graphene. Give a vector expression for the reciprocal lattice vectors $\vec{g}_1$ and $\vec{g}_2$, and sketch the reciprocal lattice.

(3) Sketch the first Brillouin zone of the lattice spanned by $\vec{g}_1$ and $\vec{g}_2$.

4.3 Linear chain with nearest-neighbor interactions

(1) Set up the equation of motion of a linear chain of N $(N \gg 1)$ identical atoms of mass m separated by a distance a and connected by springs with a spring constant f. Solve the equation using the plane wave ansatz:

$$s_n(t) = u \ \exp[i\, q\, a - \omega\, t].$$

(2) Compare the dispersion relation $\omega(q)$ obtained in (1) with that of a two-atom chain as calculated during the lecture. Use the solution of the two-atom chain to obtain the solution for a one-atom chain. Can a crystal with only a single type of atom exhibit optical phonons?

(3) Treat the elongation $s_n(t)$ as an continuous function $s(x,t)$ with $s(na,t) = s_n(t)$ and consider large wavelengths ($q \ll a^{-1}$). Show that the equation of motion obtained in (1) transforms into the wave equation of an elastic wave in a continuous medium.
Hint: Use Taylor expansions of $s((n-1)a,t)$ and $s((n+1)a,t)$.

(4) The speed of sound in a long rod is $c = \sqrt{E/\rho}$. Compare this speed of sound with that of a chain studied in (3) and determine an effective elastic modulus of the chain. Assume a simple cubic (sc) lattice and an one-atom basis for the material of the rod.