September 2, 2021

Homework 2
OPTI 507
(due September 9, 2021)

Problem 1:
Find the reciprocal lattices for the following sets of primitive translation vectors. Also state which Bravais lattice corresponds to each case, both in the original configuration space and the corresponding reciprocal space (if more than one Bravais lattice designation is possible, choose the most specific highest symmetry one).

(i)
$\vec{a} = \frac{1}{2}a(\hat{x} + \hat{y})$; $\vec{b} = \frac{1}{2}a(\hat{y} + \hat{z})$; $\vec{c} = \frac{1}{2}a(\hat{x} + \hat{z})$

(ii)
$\vec{a} = a\hat{x}$; $\vec{b} = \frac{1}{2}a\hat{x} + \frac{\sqrt{3}}{2}a\hat{y}$; $\vec{c} = c\hat{z}$

(iii)
$\vec{a} = \frac{1}{2}a(-\hat{x} + \hat{y} + \hat{z})$; $\vec{b} = \frac{1}{2}a(\hat{x} - \hat{y} + \hat{z})$; $\vec{c} = \frac{1}{2}a(\hat{x} + \hat{y} - \hat{z})$

(10 points)

Problem 2:
We define the spatial Fourier transform of a function $f(\vec{r}) = \frac{1}{(2\pi)^3}\int d^3k e^{i\vec{k}\cdot\vec{r}} f(\vec{k})$. In a crystal, certain functions, such as the charge density $\rho(\vec{r})$, are lattice periodic. Using the given form of the Fourier transform, show that, for a lattice-periodic function, $\vec{k}$ is restricted to a discrete set, defined by the conditions such as $n_1\vec{k}\cdot\vec{a} = 2\pi m_1$, etc., where n_1 and m_1 are integer numbers. Furthermore, show that the reciprocal lattice vectors, with the form of the $\vec{A}$, $\vec{B}$, $\vec{C}$ given in terms of $\vec{a}$, $\vec{b}$, $\vec{c}$ as shown in class, fulfill these conditions. For the case of a 1-dimensional crystal, make a sketch of the Brillouin zone.

(10 points)

Problem 3:
Assume you have a crystal that has the symmetry of a simple cubic Bravais lattice. Using the symmetry properties of this crystal, show that the off-diagonal matrix elements for the dielectric tensor are zero and the diagonal elements are identical. Assume all tensor elements to be real-valued. Instruction: Use the procedure presented in class, first determining the matrix elements ℓ_{ij} for a $\pi/2$ rotation about the z-axis and then similarly for a rotation about the y-axis.

(10 points)