Department of Electrical and Computer Engineering, Cornell University

ECE 4070: Physics of Semiconductors and Nanostructures

Spring 2014

Homework 2 ` **Due on Feb. 11, 2014 at 5:00 PM**

Suggested Readings:

a) Lecture notes

Problem 2.1 (Free electron gas with an anisotropic dispersion in 3D)

This problem is an exercise in calculating density of states functions that will be very useful later in the course. Suppose one has a free electron gas in 3D where the electron energy-vs-wavevector relation is given by:

$$E(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z}$$

Note that the electron has a different "mass" associated with its kinetic energy when moving in different directions. This happens in materials as a result of the interaction of the electrons with the atoms, as you will see later in the course. Find the density of states function $g(E)$ so that an integral over k-space can be converted into an integral over energy as follows:

$$2 \times \int \frac{d^3\vec{k}}{(2\pi)^3} \quad \rightarrow \quad \int_0^\infty dE \;\; g(E)$$

Hint: You can start by first defining a new wavevector $\vec{q}$ as follows:

$$q_x = \sqrt{\frac{m}{m_x}} k_x \qquad q_y = \sqrt{\frac{m}{m_y}} k_y \qquad q_z = \sqrt{\frac{m}{m_z}} k_z$$

Write the energy dispersion in terms of the wavevector components of $\vec{q}$. Convert the k-space integral into q-space integral and then convert the q-space integral into an energy integral.

Problem 2.2 (Free electron gas with an anisotropic dispersion in 2D)

Now suppose one has a free electron gas in 2D where the electron energy-vs-wavevector relation is given by:

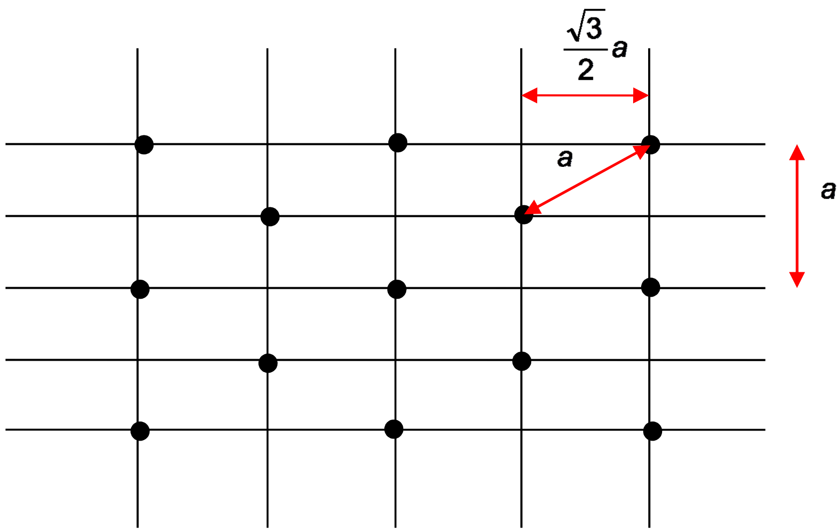
$$E(\vec{k}) = \frac{\hbar^2 k_x^2}{2m_x} + \frac{\hbar^2 k_y^2}{2m_y}$$

Find the density of states function $g_{2D}(E)$ so that an integral over k-space can be converted into an integral over energy as follows:

$$2 \times \int \frac{d^2\vec{k}}{(2\pi)^2} \quad \rightarrow \quad \int_0^\infty dE \;\; g_{2D}(E)$$

Problem 2.3 (A hexagonal lattice in 2D)

Consider the following 2D hexagonal lattice:



a) Find the primitive lattice vectors: $\vec{a}_1$ and $\vec{a}_2$.

b) Find the area of the Wigner-Seitz primitive cell.

c) Sketch, either on the homework copy or if you can draw a better diagram, the Wigner-Seitz primitive cell. Hint: it should have 6 facets.

d) Find the reciprocal lattice vectors: $\vec{b}_1$ and $\vec{b}_2$.

e) Find the area of the first Brillouin zone in k-space.

f) Plot carefully the reciprocal lattice points and the first Brillouin zone in k-space in a neat and clean diagram. Identify the reciprocal lattice type from among the 5 possible Bravais lattice types in 2D. It is important that your diagram is neat and accurately scaled otherwise your answer in part (g) will not come out right.

g) Draw enough Bragg lines on the reciprocal lattice plot of part (f) to correctly identify the first and the second Brillouin zones. On the same diagram, label all regions that belong to the first BZ and label all regions that belong to the second BZ.

h) If one is performing x-ray diffraction studies, and the incident x-ray wavevector $\vec{k}$ equals $\left(2\pi/\sqrt{3}a\right)\hat{x}$, what is the wavevector of the Bragg-scattered x-ray?

i)) If one is performing x-ray diffraction studies, and the incident x-ray wavevector $\vec{k}$ equals $\left(2\pi/\sqrt{3}a\right)\hat{x} + (2\pi/3a)\hat{y}$, what is the wavevector of the Bragg-scattered x-ray?

Problem 2.4 (FCC and BCC lattices in 3D)

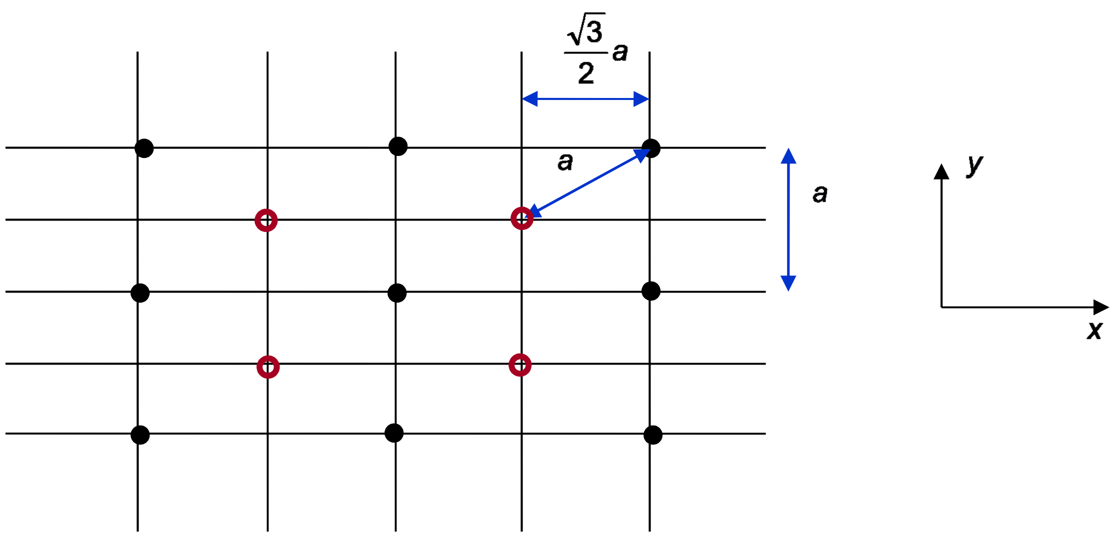
a) Show that the reciprocal lattice of the FCC lattice is the BCC lattice. Hint: Find the primitive vectors for the reciprocal lattice.

b) Show that the reciprocal lattice of the BCC lattice is the FCC lattice. Hint: Find the primitive vectors for the reciprocal lattice

c) Suppose that the lattice constant (i.e. unit cell size) of Silicon is: a = 5.43095 Angstroms. What is the density of Silicon in kg/m^3?

Problem 2.5 (A 2D lattice with a basis)

Consider the following 2D lattice made of 2 different kinds of atoms (red-unfilled and black-filled), as shown:



a) Find the primitive lattice vectors, $\vec{a}_1$ and $\vec{a}_2$, and all the basis vectors and draw them on the figure above (and submit this figure with your homework). How many basis atoms are there per lattice point?

b) Find the area of the Wigner-Seitz primitive cell of the direct lattice.

c) Sketch, on the figure above, the Wigner-Seitz primitive cell and submit it with your homework. How many atoms are there in one primitive cell?

d) Find the reciprocal lattice vectors: $\vec{b}_1$ and $\vec{b}_2$.

e) Find the area of the first Brillouin zone in k-space.

f) Sketch the reciprocal lattice points and the first Brillouin zone in k-space in a neat and clean diagram. Also draw the reciprocal lattice primitive vectors. Identify the reciprocal lattice type from among the 5 possible lattice types in 2D.