First Midterm Exam

P555

March 2, 2023

SHOW ALL WORK TO GET FULL CREDIT!

Problem 1: The array of atoms shown in Fig. 1 describe a square lattice with lattice constant a.

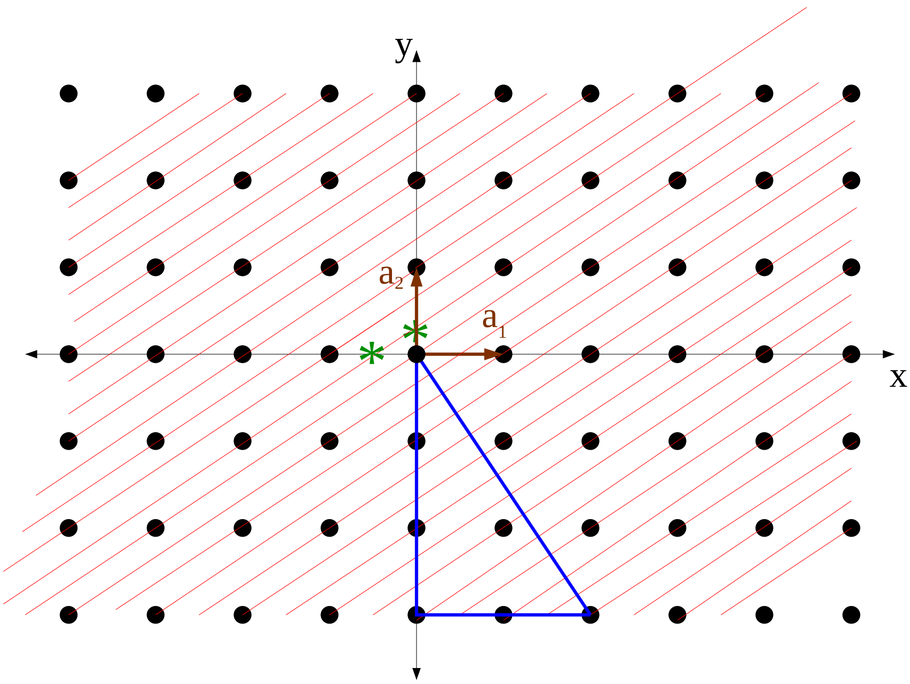

FIG. 1:

a) Provide an expression for a set of primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ in cartesian coordinates in terms of the lattice constant a and draw the vectors in Fig. 1. (5 points)

The primitive vectors are given by

$$\mathbf{a}_1 = a(1, 0) \tag{1}$$

$$\mathbf{a}_2 = a(0, 1) \tag{2}$$

b) A family of planes is indicated with red lines in Fig. 1. Provide the Miller indices for this family of planes and explain how you obtained them. (5 points)

We see that the nearest neighbor plane to the one that goes through the origin, cuts the x axis at -1/2 and the y axis at 1/3 (see green stars in the figure). Thus, the Miller indices of the planes are $(\bar{2}, 3)$.

c) Write an expression for the vector $\mathbf{K}$ in reciprocal space which is perpendicular to the family of planes in Fig. 1. (5 points)

The vector of the reciprocal lattice corresponding to the family of planes is

$$\mathbf{K} = \frac{2\pi}{a}(-2, 3). \tag{3}$$

d) What is the distance d between the planes? Explain your reasoning. (5 points)

Since $K = \frac{2\pi}{d}$ where d is the distance between nearest neighbor planes we see that $K = \frac{2\pi}{a}\sqrt{13}$. Then $d = \frac{a}{\sqrt{13}}$. We can verify this in Fig. 1 since in the blue triangle in Fig.1 we see that $13d = \sqrt{9a^2 + 4a^2} = a\sqrt{13}$. Then $d = \frac{a}{\sqrt{13}}$.

e) Now assume that x-rays with $\mathbf{k}_0 = \frac{2\pi}{a}(\frac{13}{4}, 0)$ are shone on the family of red planes. Provide the value $\mathbf{k}$, a vector, that the scatered radiation will have. Show your work. (5 points)

We know that the condition for ellastic scatering is that

$$\mathbf{k} - \mathbf{k}_0 = \mathbf{K} \tag{4}$$

and $k = k_0$. We can rewrite the expression as

$$\mathbf{k} = \mathbf{K} + \mathbf{k}_0 = \frac{2\pi}{a}(-2, 3) + \frac{2\pi}{a}(\frac{13}{4}, 0) = \frac{2\pi}{a}(\frac{5}{4}, 3). \tag{5}$$

We also see that $\mathbf{k}$ and $\mathbf{k}_0$ have the same magnitude as it corresponds to ellastic scattering since

$$k = \frac{2\pi}{a}\frac{\sqrt{169}}{4} = \frac{2\pi}{a}\frac{13}{4} = k_0. \tag{6}$$

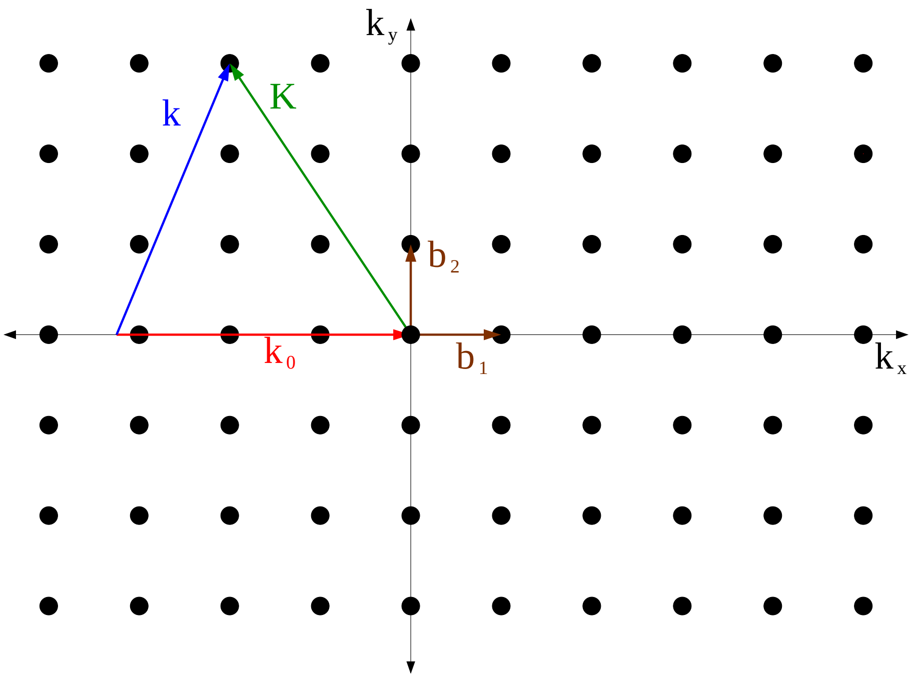

FIG. 2:

g) In Fig. 2 the points in the reciprocal space of Fig. 1 are shown. What is the separation between the nearest neighbor points in the figure? Provide your answer in terms of a. (5 points

The separation between the points is the lattice constant of the square reciprocal lattice, i.e. $b = 2\pi/a$.

h) Provide an expression for a set of primitive vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ in cartesian coordinates and draw the vectors in Fig. 2. (5 points)

The primitive vectors are given by

$$\mathbf{b}_1 = \frac{2\pi}{a}(1,0), \tag{7}$$

$$\mathbf{b}_2 = \frac{2\pi}{a}(0,1). \tag{8}$$

i) Now draw in Fig. 2 the vector $\mathbf{K}$ that you found in part (c), the vector $\mathbf{k}$ you found in part (e) and vector $\mathbf{k}_0$ provided in (e) showing that the conditions for constructive interference are satisfied by these vectors. (5 points)

Problem 2: Consider a free Fermi gas in 3 dimensions with N electrons, i.e., the electrons are free inside a cubic box of side L. Assume periodic boundary conditions.

a) Provide the values of the momentum $\mathbf{k}$ that one single electron can have. (5 points)

With PBC the allowed values of the momentum are

$$\mathbf{k} = \frac{2\pi}{L}(n_x, n_y, n_z), \tag{9}$$

with $n_i = 0, \pm1, \pm2, ...$ and $i = x, y, z$. Since the solution to the Schrödinger equation is a planewave of the form $e^{i\mathbf{k}.\mathbf{r}}$ and we need that $e^{i(k_x x + k_y y + k_z z)} = e^{i[k_x(x+L)+k_y(y+L)+k_z(z+L)]}$.

b) Provide an expression for the energy that one single electron can have. (5 points)

Since the Schrödinger equation for the free electron in a box is

$$\frac{-\hbar^2\nabla^2}{2m}\Psi = \frac{\hbar^2 k^2}{2m}\Psi = E\Psi, \tag{10}$$

we see that

$$E = \frac{\hbar^2 k^2}{2m} = \frac{4\pi^2\hbar^2(n_x^2 + n_y^2 + n_z^2)}{2mL^2}. \tag{11}$$

c) Provide the energy of the 4 lowest energy levels and indicate the degeneracy of each level. (5 points)

The lowest energy level with $(n_x, n_y, n_z) = (0,0,0)$ has $E = 0$. The second energy level has $E = \frac{4\pi^2\hbar^2}{2mL^2} = \frac{2\pi^2\hbar^2}{mL^2}$ and can be obtained with $(n_x, n_y, n_z) = (\pm1, 0, 0)$, $(0, \pm1, 0)$, or $(0, 0, \pm1)$. Thus, it has degeneracy 6. The third energy level has $E = \frac{4\pi^2\hbar^2 2}{2mL^2} = \frac{4\pi^2\hbar^2}{mL^2}$ and can be obtained with $(n_x, n_y, n_z) = (\pm1, \pm1, 0)$, $(\pm1, 0, \pm1)$, or $(0, \pm1, \pm1)$. Thus, it has degeneracy 12. The fourth energy level has $E = \frac{4\pi^2\hbar^2 3}{2mL^2} = \frac{6\pi^2\hbar^2}{mL^2}$ and can be obtained with $(n_x, n_y, n_z) = (\pm1, \pm1, \pm1)$. Thus, it has degeneracy 8.

d) Find the energy of the ground state when there are N=20 electrons inside the box. (5 points)

Each level can accommodate 2 electrons: one with spin up and one with spin down. Thus, in order to accommodate 20 electrons we place 2 in the first level, 12 in the second, and 6 in the third. The total energy is:

$$E = 2 \times 0 + 12 \times \frac{2\pi^2\hbar^2}{mL^2} + 6 \times \frac{4\pi^2\hbar^2}{mL^2} = \frac{48\pi^2\hbar^2}{mL^2}. \tag{12}$$

e) Find the Fermi energy of the system. (5 points)
The Fermi level is equal to the energy of the highest occupied level. Thus:

$$E_F = \frac{4\pi^2\hbar^2}{mL^2}. \tag{13}$$