First Midterm Exam

P555

February 25, 2021

SHOW ALL WORK TO GET FULL CREDIT!

Problem 1: Consider the array of atoms shown in Fig. 1.

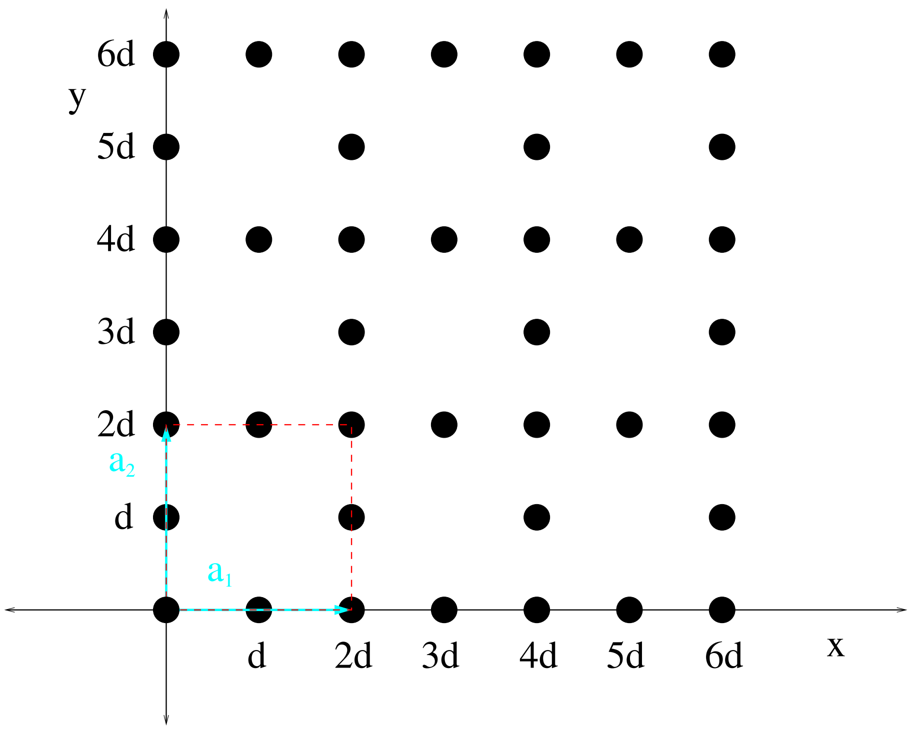

FIG. 1:

a) Draw a unit cell indicating and indicate two primitive lattice vectors in this plane.(5 points)

b) Provide an expression for the primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ that you drew in part (a), in cartesian coordinates in terms of the distance d indicated in Fig. 1. (5 points)

$$\mathbf{a}_1 = 2d(1,0), \mathbf{a}_2 = 2d(0,1). \tag{1}$$

c) How many atoms are in the unit cell? (5 points)

The total number of atoms is 3.

$$4\frac{1}{4} + 4\frac{1}{2} = 1 + 2 = 3. \tag{2}$$

d) How many points of the Bravais lattice are in the unit cell? (5 points)

The unit cell shown in the figure is a primitive cell and thus, there is only one point of the Bravais lattice in it.

e) Name the Bravais lattice. (5 points)

The Bravais lattice is a square lattice.

f) Does the system have a basis? If there is a basis provide an expression for the basis vectors in terms of the distance d indicated in the figure.(10 points)

Yes, the system has a basis. It is given by the vectors:

$$\mathbf{v}_1 = (0,0), \mathbf{v}_2 = d(1,0), \mathbf{v}_3 = d(0,1). \tag{3}$$

g) Find the primitive vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ in the reciprocal lattice. (5 points)

We know that the vectors of the reciprocal lattice have to satisfy that

$$\mathbf{a}_i.\mathbf{b}_j = 2\pi\delta_{ij}. \tag{4}$$

Then, we propose $\mathbf{b}_1 = (b_{1x}, b_{1y})$ and $\mathbf{b}_2 = (b_{2x}, b_{2y})$ and we solve for b_{1x}, b_{1y}, b_{2x}, and b_{2y} in the equations:

$$2\pi = \mathbf{a}_1.\mathbf{b}_1 = 2db_{1x}, 0 = \mathbf{a}_2.\mathbf{b}_1 = 2db_{1y}, 0 = \mathbf{a}_1.\mathbf{b}_2 = 2db_{2x}, 2\pi = \mathbf{a}_2.\mathbf{b}_2 = 2db_{2y}. \tag{5}$$

We obtain:

$$\mathbf{b}_1 = \frac{2\pi}{2d}(1,0) = \frac{\pi}{d}(1,0), \mathbf{b}_2 = \frac{2\pi}{2d}(0,1) = \frac{\pi}{d}(0,1). \tag{6}$$

h) Calculate the modulation factor $F_{\mathbf{K}}$. (10 points)

A generic vector of the reciprocal lattice is given by

$$\mathbf{K} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 = \frac{\pi}{d}(n_1, n_2), \tag{7}$$

where n_1 and n_2 are integers. The next step is to calculate $\mathbf{v}_i.\mathbf{K}$:

$$\mathbf{v}_1.\mathbf{K} = (0,0), \mathbf{v}_2.\mathbf{K} = d(1,0).\frac{\pi}{d}(n_1,n_2) = \pi n_1, \mathbf{v}_3.\mathbf{K} = d(0,1).\frac{\pi}{d}(n_1,n_2) = \pi n_2. \tag{8}$$

Then the modulation factor is given by:

$$F_{\mathbf{K}} = |1 + e^{i(\mathbf{v}_2.\mathbf{K})} + e^{i(\mathbf{v}_3.\mathbf{K})}|^2 = |1 + e^{i\pi n_1} + e^{i\pi n_2}|^2. \tag{9}$$

i) Find the posible values of $F_{\mathbf{K}}$ and say if it describes an interference pattern from a Bravais lattice or from a Bravais lattice with a basis. Explain. (5 points)

From Eq. 9 we see that $F_{\mathbf{K}} = 9$ if n_1 and n_2 are even and $F_{\mathbf{K}} = 1$ otherwise. Thus, we see that thanks to the presence of atoms in a basis some interference points are enhanced and have an intensity which is 9 times the value that they had in a lattice without a basis.

j) Now some of the black atoms are replaced by two different kind of atoms, red and green as shown in Fig. 2. Draw the unit cell in this new situation.(5 points)

k) Provide an expression for the primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ in cartesian coordinates in terms of the distance d indicated in Fig. 2. (5 points)

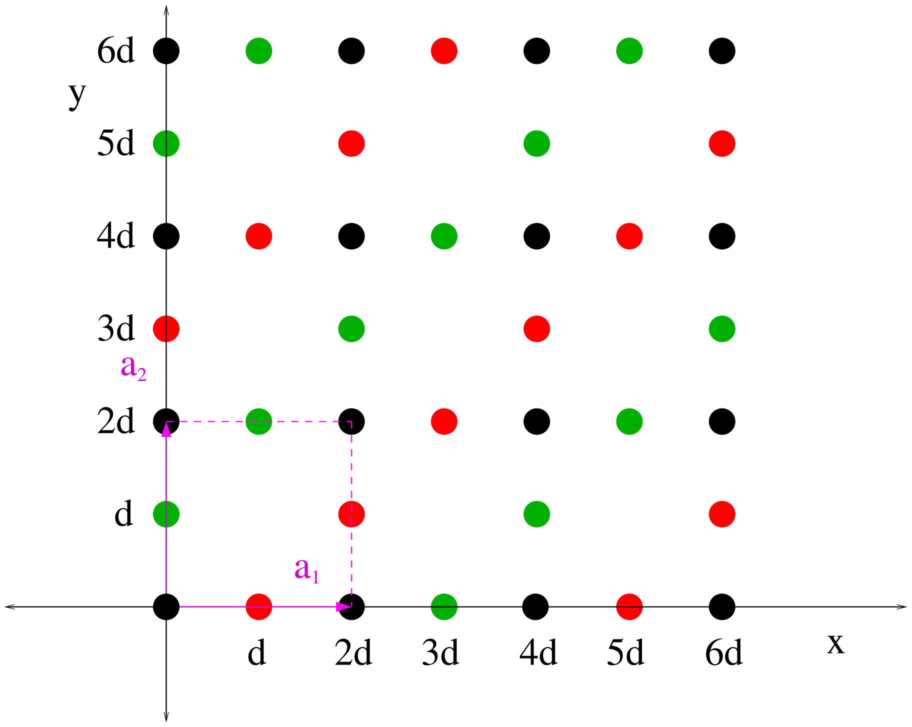

FIG. 2:

Notice that the only thing that has changed with respect to part (a) and (b) is that the color of the atoms has changed. Thus the primitive unit clell is the same and the primitive vectors are the same

$$\mathbf{a}_1 = 2d(1,0), \mathbf{a}_2 = 2d(0,1). \tag{10}$$

l) How many atoms are in the unit cell? (5 points)

As in (c) there are still 3 atoms in the primitive unit cell.
The number of black atoms is given by:

$$4\frac{1}{4} = 1. \tag{11}$$

The number of red atoms is 1/2+1/2=1 and the number of green atoms is also 1/2+1/2=1.

m) How many points of the Bravais lattice are in the unit cell? (5 points)

The Bravais lattice contains one single lattice point.

n) Name the Bravais lattice. (5 points)

The Bravais lattice is a square lattice with lattice constant $a = 2d$.

o) Does the system have a basis? If there is a basis provide an expression for the basis vectors in terms of the distance d indicated in the figure.(10 points)

Yes, the system has a basis.

For the black atoms it is given by the vector:

$$\mathbf{v}_1 = (0, 0), \tag{12}$$

For the green atoms it is given by the vector:

$$\mathbf{v}_2 = d(1, 0), \tag{13}$$

For the red atoms it is given by the vector:

$$\mathbf{v}_3 = d(0, 1), \tag{14}$$

p) Find the primitive vectors $\mathbf{b}_1$ and $\mathbf{b}_2$ in the reciprocal lattice. (5 points)

They are the same as in part (g). Thus

$$\mathbf{b}_1 = \frac{\pi}{d}(1, 0), \mathbf{b}_2 = \frac{\pi}{d}(0, 1). \tag{15}$$

q) Name one symmetry present in the monoatomic system shown in Fig. 1 that is lost when red and green atoms are introduced as in Fig. 2. (5 points)

The lattice in Fig. 1 is invariant under rotations by $\pi/2$ about a point in the Bravais lattice. That symmetry is lost when the red and green atoms are introduced. Other symmetries that are lost: Reflections along a diagonal (45 degrees from the x-axis) (notice that reflections about the diagonal that makes a 135 degrees angle with the x-axis are conserved); reflexions about the x-axis; reflections about the y-axis.