P555
February 13, 2020

SHOW ALL WORK TO GET FULL CREDIT!

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

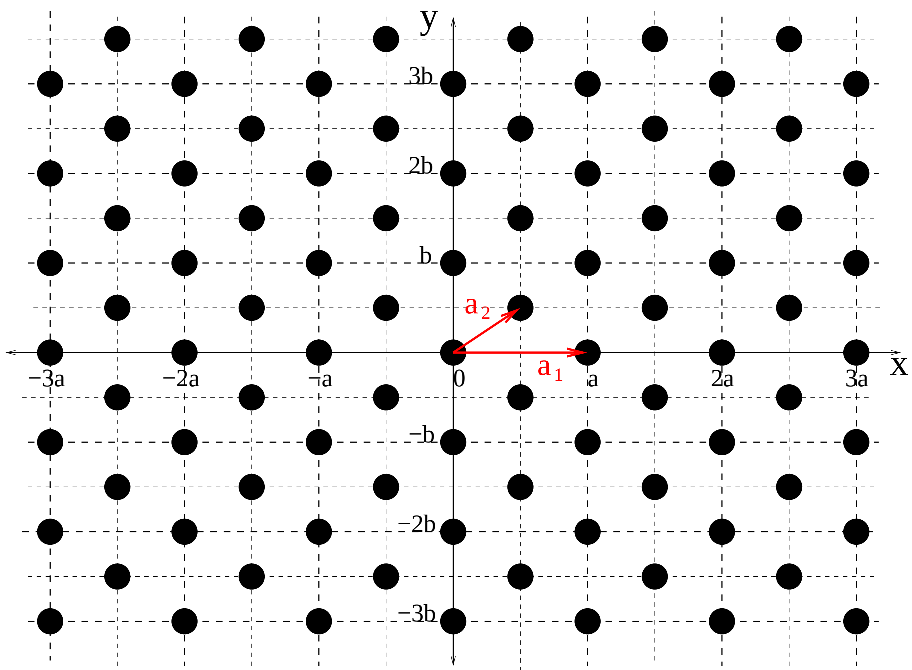

FIG. 1:

a) Explain why the points form a Bravais lattice and name (provide the name of) the lattice.(5 points)

The points in the figure form a Bravais lattice because each atom at each site of the lattice is surrounded by an identical array of atoms, i.e., each black atom is surrounded by 4 black atoms located at a distance $d = \pm a/2, \pm b/2)$. The Bravais lattice is thus, centered rectangular because there is an atom at the center of each rectangle of sides a and b.

b) Provide a set of primitive vectors for this lattice. Draw the vectors in Fig. 1 and write an expression for them in cartesian coordinates in terms of the constants a and b.(5 points)

A possible set of primitive vectors is given by

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

c) Find the primitive vectors for the reciprocal lattice of the Bravais lattice shown in Fig. 1. Provide an expression for them in cartesian coordinates in terms of the constants a and b. (5 points)

To obtain the reciprocal lattice vectors we know that

$$\mathbf{b}_1.\mathbf{a}_1 = 2\pi = b_{1,x}a, \tag{2}$$

which means that

$$b_{1,x} = \frac{2\pi}{a}. \tag{3}$$

We also know that

$$\mathbf{b}_1.\mathbf{a}_2 = 0 \tag{4}$$

which means that

$$0 = b_{1,x}\frac{a}{2} + b_{1,y}\frac{b}{2} = \pi + b_{1,y}\frac{b}{2}, \tag{5}$$

which means that

$$b_{1,y} = -\frac{2\pi}{b}. \tag{6}$$

Then

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

We also know that

$$\mathbf{b}_2.\mathbf{a}_1 = 0 \tag{8}$$

which means that

$$0 = b_{2,x}\frac{a}{2} \tag{9}$$

which means that

$$b_{2,x} = 0. \tag{10}$$

We also know that

$$\mathbf{b}_2.\mathbf{a}_2 = 2\pi = b_{2,x}\frac{a}{2} + b_{2,y}\frac{b}{2} = b_{2,y}\frac{b}{2}, \tag{11}$$

which means that

$$b_{2,y} = \frac{4\pi}{b}. \tag{12}$$

Then

$$\mathbf{b}_2 = (0, \frac{4\pi}{b}). \tag{13}$$

d) Draw the vectors found in part (c) in Fig. 2 and identify (provide the name of) the Bravais lattice that they generate.(5 points)

The Bravais lattice in reciprocal space is centered rectangular.

e) In cartesian coordinates provide an expression for a generic vector $\mathbf{K}$ in reciprocal space and indicate with a circle in Fig. 2 the end point of all the reciprocal vectors that fit in the figure (Hint: verify that the points you draw agree with the answer you provided in (d)). (5 points)

The generic vector in reciprocal space is given by

$$\mathbf{K} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 = (n_1\frac{2\pi}{a}, -n_1\frac{2\pi}{b} + n_2\frac{4\pi}{b}) = (n_1\frac{2\pi}{a}, (2n_2 - n_1)\frac{2\pi}{b}), \tag{14}$$

where $n_i = 0, \pm 1, \pm 2, ...$

Problem 2: Consider the array of atoms shown in Fig. 3.

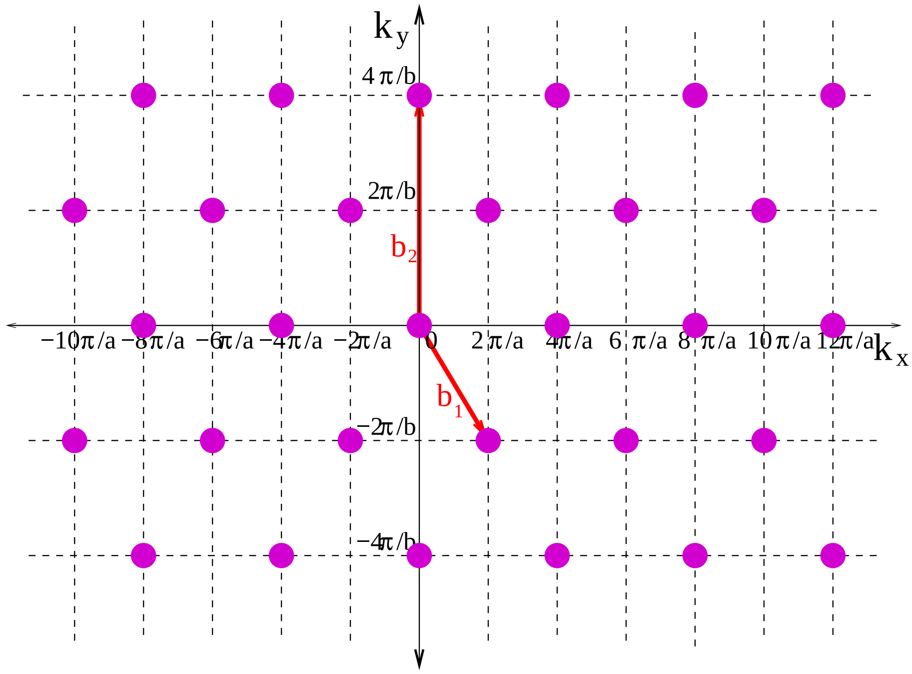

FIG. 2:

a) Are all the atoms in the figure sitting at the sites of a Bravais lattice or is this system represented by a Bravais lattice with a basis? Justify your answer. (5 points)

The points in the figure do not form a Bravais lattice because each atom is not surrounded by an identical array of atoms, i.e., each black atom is surrounded by 4 white atoms located at a distance $d = \pm a/2, \pm b/2)$ while each white atom is surrounded by 4 black atoms located at a distance $d = \pm a/2, \pm b/2)$. Thus, this array is represented by a Bravais lattice defined by the black atoms and a basis that accounts for the white atoms.

b) Name (provide the name of) the Bravais lattice and, if needed, provide a set of basis vectors (in cartesian coordinates and in terms of a and b) and draw the basis in Fig. 3. (5 points)

We see that the black atoms are at the sites of a rectangular Bravais lattice with basis vectors:

$$\mathbf{v}_1 = (0,0),\ \mathbf{v}_2 = (\frac{a}{2}, \frac{b}{2}). \tag{15}$$

c) Provide a set of primitive vectors for the Bravais lattice. Draw the vectors in Fig. 3 and write an expression for them in cartesian coordinates in terms of the constants a and b. (5 points)

A possible set of primitive vectors is given by:

$$\mathbf{a}_1 = a(1,0),\ \mathbf{a}_2 = b(0,1). \tag{16}$$

d) Find the primitive vectors for the reciprocal lattice of the Bravais lattice shown in Fig. 3. Provide an expression for them in cartesian coordinates in terms of the constants a and b. (5 points)

To obtain the reciprocal lattice vectors we know that

$$\mathbf{b}_1.\mathbf{a}_1 = 2\pi = b_{1,x}a, \tag{17}$$

which means that

$$b_{1,x} = \frac{2\pi}{a}. \tag{18}$$

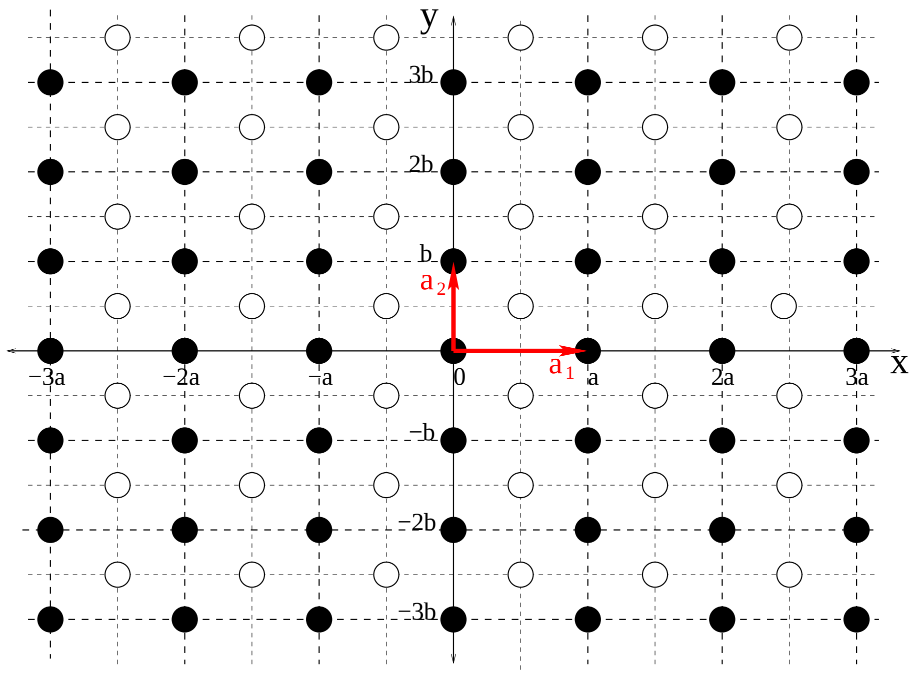

FIG. 3:

We also know that

$$\mathbf{b}_1.\mathbf{a}_2 = 0 \tag{19}$$

which means that

$$0 = b_{1,y}b, \tag{20}$$

which means that

$$b_{1,y} = 0. \tag{21}$$

Then

$$\mathbf{b}_1 = (\frac{2\pi}{a}, 0). \tag{22}$$

We also know that

$$\mathbf{b}_2.\mathbf{a}_1 = 0 \tag{23}$$

which means that

$$0 = b_{2,x}a \tag{24}$$

which means that

$$b_{2,x} = 0. \tag{25}$$

We also know that

$$\mathbf{b}_2.\mathbf{a}_2 = 2\pi = b_{2,y}b \tag{26}$$

which means that

$$b_{2,y} = \frac{2\pi}{b}. \tag{27}$$

Then

$$\mathbf{b}_2 = (0, \frac{2\pi}{b}). \tag{28}$$

e) Draw the vectors found in part (d) in Fig. 4 and identify (provide the name of) the Bravais lattice that they generate. (5 points)

We see that the Bravais lattice in reciprocal space is rectangular.

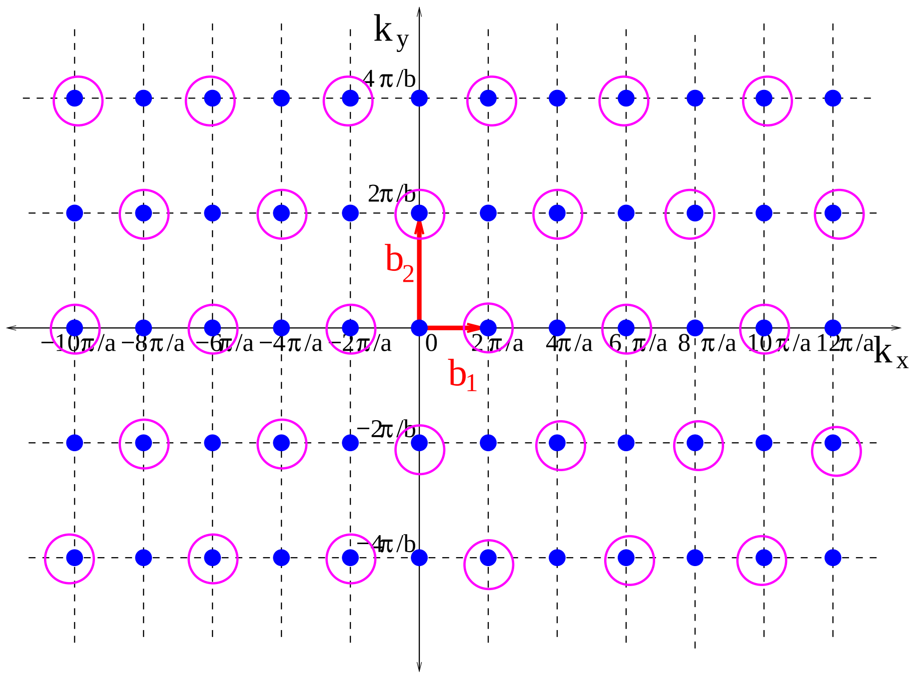

FIG. 4:

f) In cartesian coordinates provide an expression for a generic vector **K** in reciprocal space and indicate with a circle in Fig. 4 the end point of all the reciprocal vectors that fit in the figure (Hint: verify that the points you draw agree with the answer you provided in (e)). (5 points)

The generic vector in reciprocal space is given by

$$\mathbf{K} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 = (n_1\frac{2\pi}{a} + n_2\frac{2\pi}{b}), \tag{29}$$

where $n_i = 0, \pm 1, \pm 2, ...$

g) Now assume that the white atoms in Fig. 3 are replaced by black atoms, i.e., all the atoms in the figure are now identical. Calculate the modulation factor $F_{\mathbf{k}}$. (5 points)

We know that the modulation factor is given by

$$F_{\mathbf{k}} = |\sum_{l=1}^{N} e^{-i\mathbf{K}.\mathbf{v}_l}|^2. \tag{30}$$

In our case $N = 2$. As we saw in (f) the generic vector in reciprocal space is given by $\mathbf{K} = (n_1\frac{2\pi}{a}, n_2\frac{2\pi}{b})$. We see that $\mathbf{K}.\mathbf{v}_1 = 0$ and

$$\mathbf{K}.\mathbf{v}_2 = (n_1\frac{2\pi}{a}, n_2\frac{2\pi}{b}).(\frac{a}{2}, \frac{b}{2}) = (n_1 + n_2)\pi. \tag{31}$$

Then,

$$F_{\mathbf{k}} = |1 + e^{-i(n_1+n_2)\pi}|^2. \tag{32}$$

h) Find an expression for the zeroes in $F_{\mathbf{k}}$. (5 points)
We see that $F_{\mathbf{k}} = 0$ when $(n_1 + n_2) = 2n + 1$, i.e. an odd number.

i) In Fig. 4 draw a circle around the points in reciprocal space for which $F_{\mathbf{k}} = 0$. (5 points)

j) Compare the pattern you obtained in Fig. 4 with the points in Fig. 2. What would you expect? Does the result you found match your expectations? (5 points)
We see that the surviving points are the same that we found in part (e) of problem one because when the white atoms are replaced by black ones the lattice of problem 2 becomes identical to the one in problem one and we expect to see that it really is now a centered rectangular lattice.