P555

March 3, 2022

SHOW ALL WORK TO GET FULL CREDIT!

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

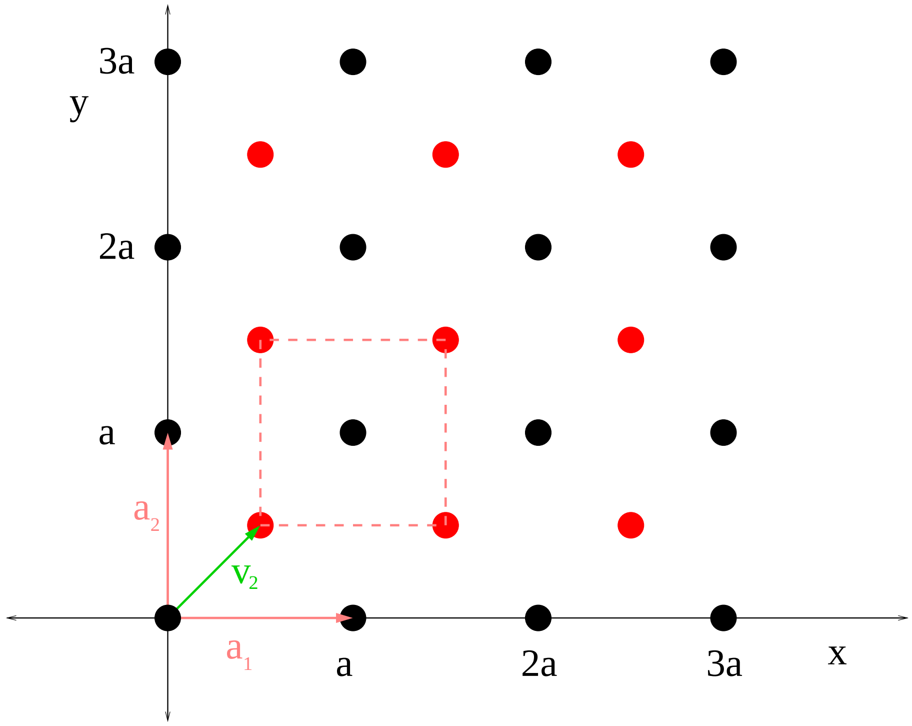


FIG. 1:

a) What is the Bravais lattice?(5 points)

The Bravais lattice is square with lattice constant $a$.

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

The primitive vectors are given by

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

c) Draw a primitive unit cell in Fig. 1. (5 points)

See Fig. 1.

d) How many atoms are in the primitive unit cell that you drew? (5 points)

We see that there are two different atoms in the primitive cell: one black atom at the center (Bravais lattice point) and one quarter of the 4 red atoms at the vertices of the cell, making one red atom in the cell.

e) How many points of the Bravais lattice are in the primitive unit cell that you drew? (5 points)

There is only one point of the Bravais in the primitive unit cell. This is expected because a primitive cell should contain only one Bravais lattice point.

f) Do you need to provide a basis to represent the structure in Fig. 1? If you need a basis provide an expression for the basis vectors in terms of the distance $a$ indicated in the figure.(5 points)

Yes, we need to provide a basis due to the presence of the red atoms. The basis is given by

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

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

The primitive vectors of the reciprocal lattice satisfy $\mathbf{a}_i.\mathbf{b}_j = \delta_{i,j}$ and thus, they are given by:

$$\mathbf{b}_1 = \frac{2\pi}{a}(1,0), \mathbf{b}_2 = \frac{2\pi}{a}(0,1). \tag{3}$$

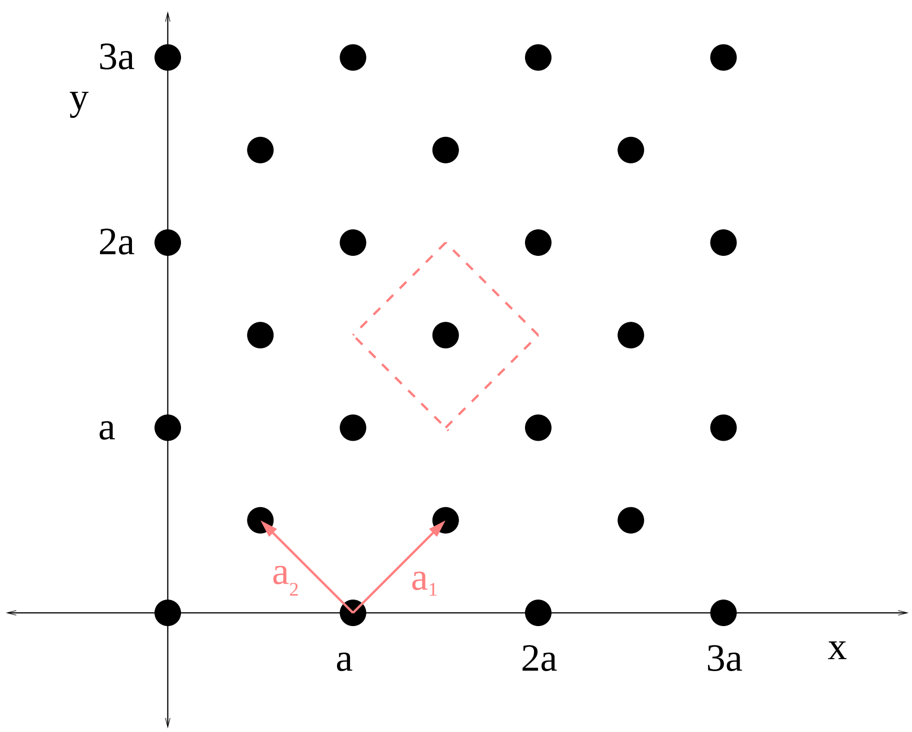


FIG. 2:

h) Now the red atoms are replaced by black atoms so that all the atoms in the material are the same as shown in Fig. 2. Calculate the modulation factor $F_{\mathbf{K}}$ if you provided a basis in part (f). (5 points)

The modulation factor is given by

$$F_{\mathbf{k}} = |\sum_{l=1}^{n} e^{i\mathbf{K}.\mathbf{v}_l}|^2, \tag{4}$$

where $n$ is the number of vectors in the basis. In this case $n = 2$ and $\mathbf{K} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 = \frac{2\pi}{a}(n_1, n_2)$ is a generiac vector of the reciprocal lattice. We see that $\mathbf{K}.\mathbf{v}_1 = 0$ and

$$\mathbf{K}.\mathbf{v}_2 = \pi(n_1 + n_2). \tag{5}$$

Then,

$$F_{\mathbf{k}} = |\sum_{l=1}^{2} e^{i\mathbf{K}.\mathbf{v}_l}|^2 = |1 + e^{i\pi(n_1+n_2)}|^2. \tag{6}$$

i) Under what conditions $F_{\mathbf{K}} = 0$? Provide a vector of the reciprocal lattice for which the modulation factor vanishes.(5 points)

We see that $F_{\mathbf{K}} = 0$ if $n_1 + n_2 = 2r + 1$ with r an integer, i.e., the sum of both indices has to be an odd number. A vector of the reciprocal lattice that satisfies this could be $\mathbf{K} = \frac{2\pi}{a}(1, 2)$.

j) For the lattice shown in Fig. 2 with all the atoms being the same, draw a primitive unit cell in Fig. 2.(5 points)

See Fig. 2.

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

$$\mathbf{a}'_1 = \frac{a}{2}(1, 1), \mathbf{a}'_2 = \frac{a}{2}(-1, 1). \tag{7}$$

The Bravais lattice is square.

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

There is one atom in the primitive cell.

m) Does this lattice need a basis? If the answer is yes, provide the basis (5 points)

This lattice does not need a basis.

**Problem 2**: Consider a free Fermi gas in 2 dimensions with N electrons, i.e., the electrons are free inside a square 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

$$\mathbf{k} = \frac{2\pi}{L}(n_x, n_y), \tag{8}$$

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

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

$$\frac{-\hbar^2\nabla^2}{2m}\Psi = \frac{\hbar^2 k^2}{2m}\Psi = E\Psi, \tag{9}$$

we see that

$$E = \frac{\hbar^2 k^2}{2m} = \frac{4\pi^2\hbar^2(n_x^2 + n_y^2)}{2mL^2}. \tag{10}$$

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

The lowest energy level with $(n_x, n_y) = (0, 0)$ 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 $(n_x, n_y) = (\pm 1, 0)$ or $(0, \pm 1)$. Thus, it has degeneracy 4. 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 $(n_x, n_y) = (\pm 1, \pm 1)$. Thus, it has degeneracy 4. The fourth energy level has $E = \frac{4\pi^2\hbar^2 4}{2mL^2} = \frac{8\pi^2\hbar^2}{mL^2}$ and can be obtained with $(n_x, n_y) = (\pm 2, 0)$ or $(0, \pm 2)$. Thus, it has degeneracy 4.

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, 8 in the second, 8 in the third, and 2 in the fourth. The total energy is:

$$E = 2 \times 0 + 8 \times \frac{2\pi^2\hbar^2}{mL^2} + 8 \times \frac{4\pi^2\hbar^2}{mL^2} + 2 \times \frac{8\pi^2\hbar^2}{mL^2} = \frac{48\pi^2\hbar^2}{mL^2}. \tag{11}$$