First Midterm Exam

P555

February 29, 2024

SHOW ALL WORK TO GET FULL CREDIT!

Problem 1: Fig. 1 shows an array of two different kinds of atoms in real space: black and red. The axis of coordinates are shown.

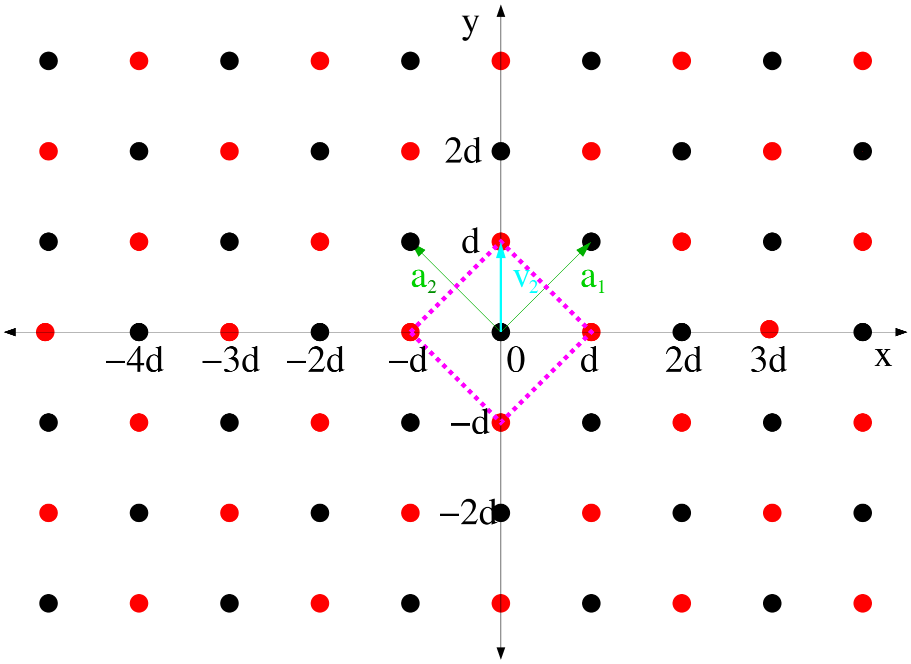

FIG. 1:

a) What is the two dimensional Bravais lattice in which the atoms in Fig. 1 are arranged? Provide the lattice constants in terms of the distance d. (5 points)

The Bravais lattice is a square lattice with lattice constant $a = \sqrt{2}d$.

b) Provide an expression for a set of primitive vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ in cartesian coordinates in terms of the length d shown in the figure and draw the vectors in Fig. 1. (10 points)

A set of primitive vectors is given by

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

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

The vectors are drawn in green in Fig. 1.

c) Draw a primitive unit cell and indicate how many atoms and how many points of the Bravais lattice are inside the cell. Justify your answer. (5 points)

The primitive unit cell is indicated with a dashed magenta line in Fig. 1. We see that there are two atoms inside the cell: 1 black and 1 red, since each of the 4 red atoms is shared between 4 primitive cells.

d) Explan why a basis is needed to describe the array of atoms shown in Fig. 1, provide an expression for the basis vectors, and draw them in the figure. (10 points)

A basis is needed because there are two types of atoms black and red. Notice that if all atoms were the same, i.e. black, we would have a square Bravais lattice with lattice constant $a = d$. Since there are two atoms inside a primitive unit cell we need two basis vectors:

$$\mathbf{v}_1 = (0, 0) \tag{3}$$

for black atoms and

$$\mathbf{v}_2 = d(0, 1) \tag{4}$$

for red atoms. Vector $\mathbf{v}_2$ is drawn in light blue in Fig. 1.

e) Find a basis for the reciprocal lattice corresponding to the Bravais lattice that you found in part (b). Draw the basis vectors in Fig. 2 and label each tick mark in Fig. 2 in terms of the length d provided in Fig. 1. The dashed lines in Fig. 2 are provided to help you in your drawings.(10 points)

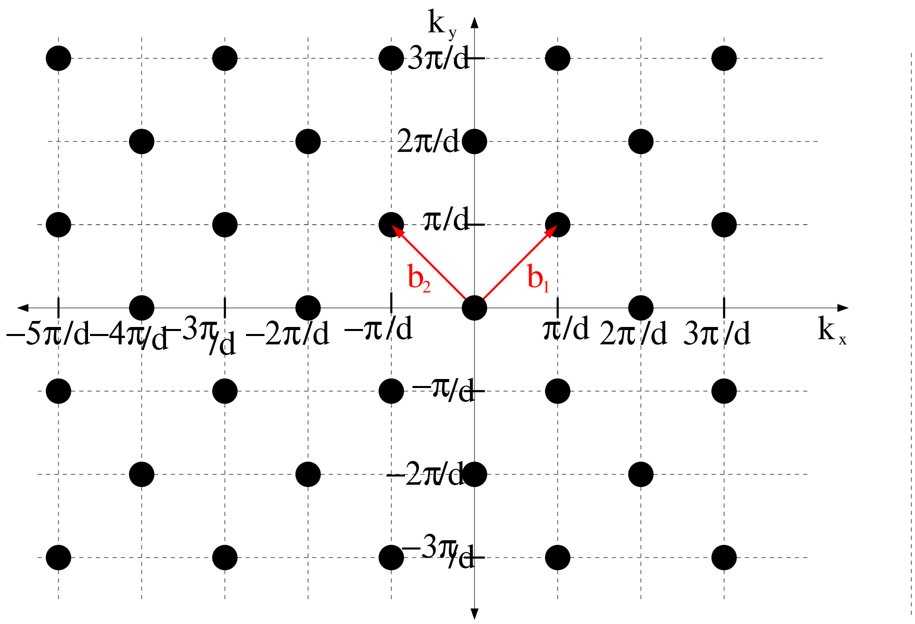

FIG. 2:

A set of primitive vectors of the reciprocal lattice is given by

$$\mathbf{b}_1 = \frac{\pi}{d} d(1, 1) \tag{5}$$

$$\mathbf{b}_2 = \frac{\pi}{d}(-1, 1) \tag{6}$$

The vectors are draw in red in Fig. 2. We can see that the vectors provided satisfy that $\mathbf{a}_i.\mathbf{b}_j = 2\pi\delta_{i,j}$.

f) Write an expression for a generic vector $\mathbf{K}$ in reciprocal space and indicate with black dots in Fig. 2 all the vectors of the reciprocal lattice that fit in the figure. The dashed lines in Fig. 2 are provided to help you in your drawings. (10 points)

A generic vector in the reciprocal lattice is given by

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

where n_i are integers. The black points in Fig. 2 indicate all the reciprocal lattice vectors that fit in it.

g) Now assume that the red atoms in Fig. 1 are identical to the black atoms and provide an expression for the modulation factor $F_{\mathbf{K}}$. (5 points)

We know that the modulation factor is given by

$$F_{\mathbf{K}} = |\sum_l e^{i\mathbf{K}.\mathbf{v}_l}|^2 \tag{8}$$

In our case $\mathbf{K}.\mathbf{v}_1 = 0$ and

$$\mathbf{K}.\mathbf{v}_2 = \frac{\pi}{d}(n_1 - n_2, n_1 + n_2).d(0, 1) = \pi(n_1 + n_2), \tag{9}$$

then,

$$F_{\mathbf{K}} = |1 + e^{i\pi(n_1+n_2)}|^2 \tag{10}$$

h) Are there points in the diffraction pattern that you drew in Fig. 2 that will vanish? If this is the case indicate which points will vanish and draw in Fig. 3 the points that survive. (10 points)

The modulation factor vanishes when $n_1 + n_2$ is odd. This happens if n_1 is even (odd) and n_2 is odd (even). These points, which will vanish, are indicated with open circles in Fig. 3.

Bonus) What does the difraction pattern that you drew in Fig. 3 indicate about the Bravais lattice in Fig. 1 when the red atoms are replaced by black atoms? Explain. Hint: think about what is the Bravais lattice in this situation, and what are the primitive vectors. (10 points)

We see that the points in Fig. 3 correspond to a square reciprocal lattice with lattice constant $\frac{2\pi}{d}$, as indicated by the blue primitive vectors $\mathbf{b'}_i$ in Fig. 3, which is what we would expect because when the red atoms are replaced by black ones the original lattice in Fig. 1 becomes a square Bravais lattice with latice constant $a = d$.

Problem 2: Consider a free Fermi gas in 3 dimensions with N electrons. The electrons are free inside a box with a square bottom of side L and a height $2L$. Assume periodic boundary conditions.

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

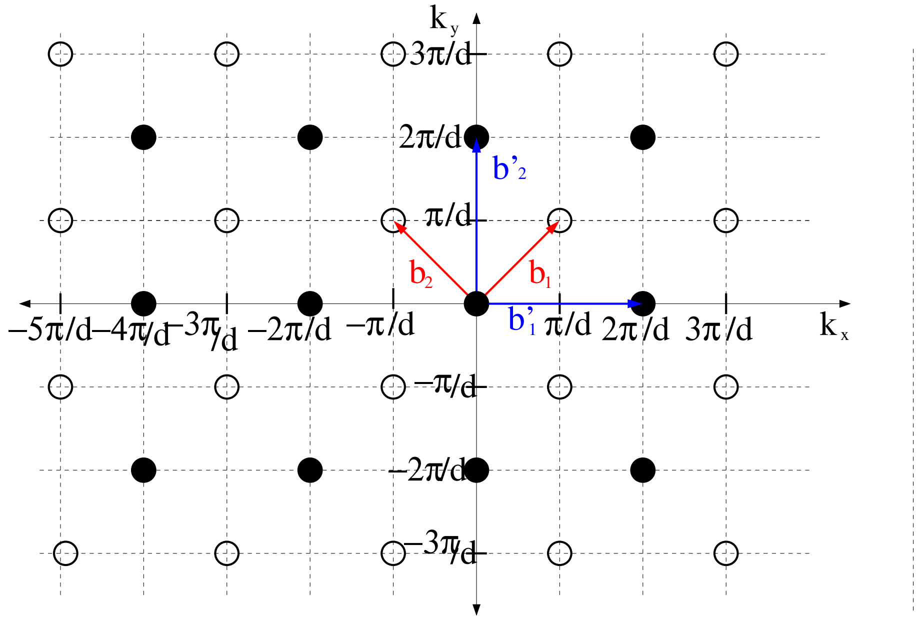

FIG. 3:

Using the boundary conditions we know that

$$k_x = \frac{2\pi n_x}{L}, \tag{11}$$

with $n_x = 0, \pm 1, \pm 2, \ldots$.

$$k_y = \frac{2\pi n_y}{L}, \tag{12}$$

with $n_y = 0, \pm 1, \pm 2, \ldots$.

$$k_z = \frac{2\pi n_z}{2L}, \tag{13}$$

with $n_z = 0, \pm 1, \pm 2, \ldots$.

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

The energy of a free electron is $p^2/2m$ and it is thus given by

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m} = \frac{\hbar^2 \pi^2 (4n_x^2 + 4n_y^2 + n_z^2)}{2mL^2} = \frac{h^2 (4n_x^2 + 4n_y^2 + n_z^2)}{8mL^2}. \tag{14}$$

with $n_i = 0, \pm 1, \pm 2, \ldots$.

c) Provide the energy of the 4 lowest energy levels and indicate the degeneracy of each level and make a figure indicating each of the 4 levels and its degeneracy. (10 points)

The lowest energy level is given by $(n_x, n_y, n_z) = (0, 0, 0)$, followed by $(0, 0, \pm 1)$ with degeneracy 2. Then we notice that $(0, 0, \pm 2)$, $(\pm 1, 0, 0)$, and $(0, \pm 1, 0)$ have all the same energy, i.e. the third level has degeneracy 6, and the fourth level is given by $(\pm1, 0, \pm1)$, and $(0, \pm1, \pm1)$ and it has degeneracy 8. The levels, their energies, in units of $\frac{h^2}{8mL^2}$, and their degeneracies are indicated in Fig. 4.

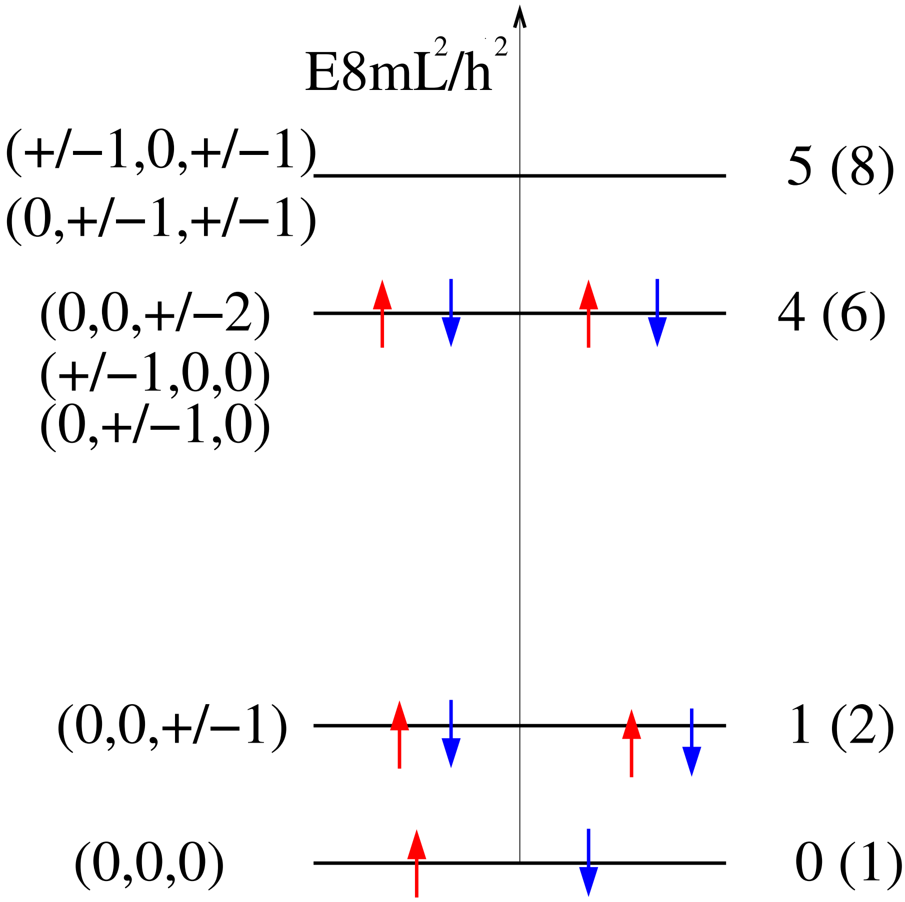

FIG. 4:

d) Find the energy of the ground state when there are N=10 electrons inside the box. Place the 10 electrons in the energy levels that you drew in part (c). (10 points)

If we have 10 electrons we will fill up to the first 3 levels as it can be seen in Fig. 4. The total energy of the system is

$$E = \frac{h^2(2 \times 0 + 4 \times 1 + 4 \times 4)}{8mL^2} = \frac{5h^2}{2mL^2}. \tag{15}$$

e) Find the Fermi energy of the system. (5 points)

The Fermi energy of the system is given by the energy of the third level:

$$E_F = E(0, 0, 2) = \frac{\hbar^2\pi^2(0 + 0 + 4)}{2mL^2} = \frac{h^2}{2mL^2}. \tag{16}$$