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Problem 1: A two dimensional metal has one atom of valency one in a simple rectangular primitive cell with lattice constants $a = 2\text{\AA}$ and $b = 4\text{\AA}$.

a) Find a set of primitive vectors for the reciprocal lattice and provide their length in cm^{-1} . (5 points)
The primitive vectors are

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

Since $a = 2\text{\AA} = 2 \times 10^{-8} \text{ cm}$, we see that $b_1 = 31.4 \times 10^7 \text{ cm}^{-1}$ and since $b = 4\text{\AA} = 4 \times 10^{-8} \text{ cm}$, we see that $b_2 = 15.7 \times 10^7 \text{ cm}^{-1}$

b) Make a plot of the first Brillouin and provide its dimensions in cm^{-1} . (5 points)

See Fig. 1 for the FBZ indicated in red. We see that it is a rectangle that extends from $-\pi/a$ to π/a along x with $\pi/a = 15.7 \times 10^7 \text{ cm}^{-1}$ and from $-\pi/b$ to π/b along y with $\pi/b = 7.85 \times 10^7 \text{ cm}^{-1}$.

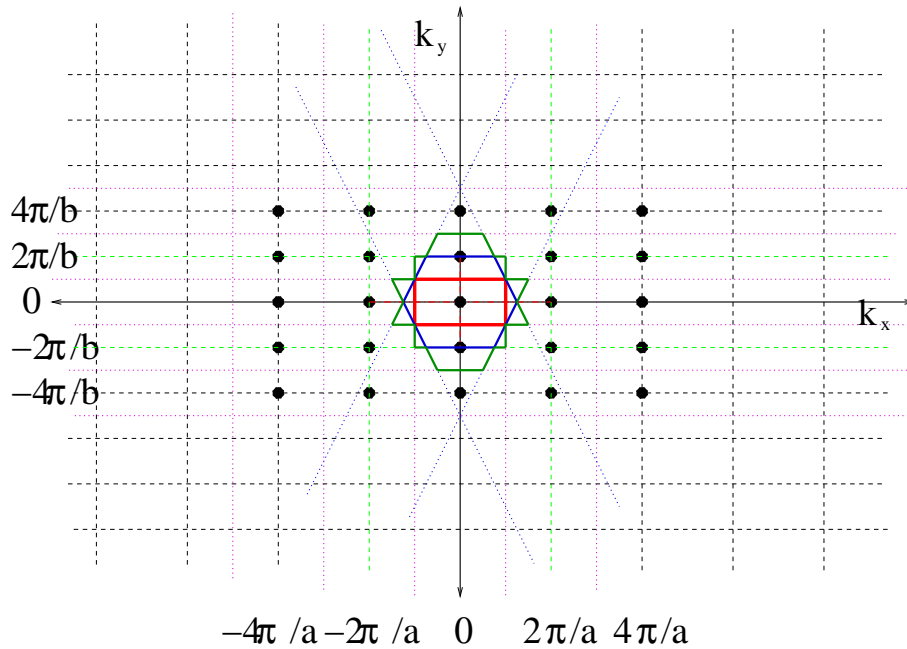


FIG. 1: The FBZ is indicated in red, the second in blue, and the third in green.

c) Add the second and third Brillouin zones to your plot. (5 points)

See Fig. 1.

d) Calculate the radius of the free fermion electron Fermi sphere (circle in 2D) in cm^{-1} at $T = 0$. (5 points)

We need to perform a calculation similar to the one we did in class to find the radius of the Fermi sphere in 3D but remembering that now we are in 2D.

We know that the total number of electrons will be given by

$$N = A \int_0^\infty \frac{2}{(2\pi)^2} \theta(k_F - k) d^2k = A \frac{2\pi \cdot 2}{(2\pi)^2} \int_0^{k_F} k dk = \frac{A}{2\pi} k_F^2, \tag{2}$$

where $A = ab$ is the area of the unit cell in real space. Then,

$$k_F = \sqrt{\frac{2\pi N}{A}} = \sqrt{2\pi n}. \quad (3)$$

For a monovalent metal $N = 1$ and in our case $A = 8 \times 10^{-16} \text{ cm}^2$ then we obtain:

$$k_F = \sqrt{\frac{2\pi}{A}} = 8.86 \times 10^7 \text{ cm}^{-1}. \quad (4)$$

- e) Draw this sphere to scale on your drawing of the Brillouin zones. (5 points)
The sphere is indicated with a brown line in Fig. 2.

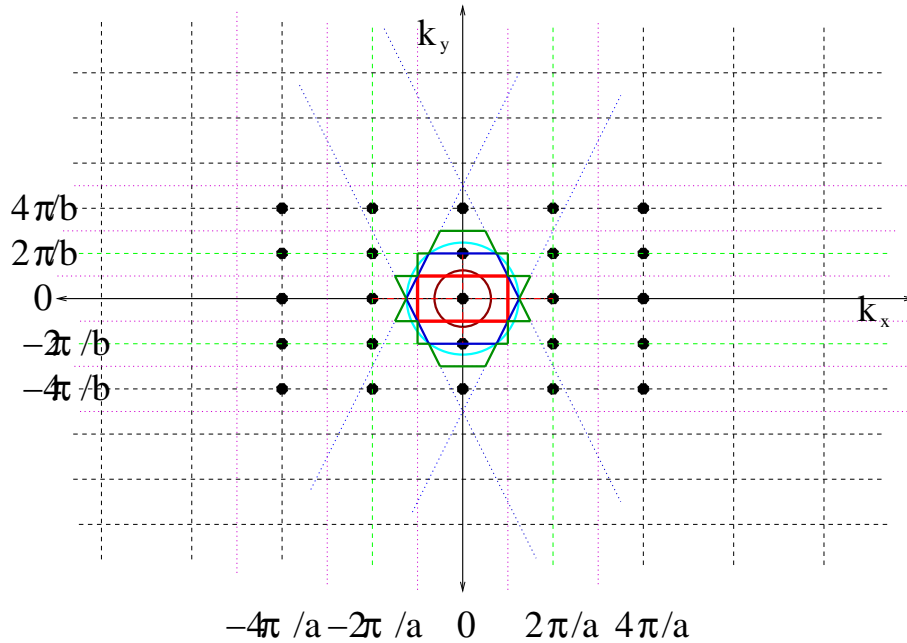


FIG. 2: The FBZ is indicated in red, the second in blue, and the third in green. The free electron FS for a monovalent metal is indicated in brown and the one for a metal with valency 4 is indicated in light blue.

- f) Indicate the occupation of the first, second, and third Brillouin zones, i.e. say if the zones are occupied or empty. (5 points)

As we can see in the figure the first and second BZ are partially occupied while the third one is empty.

- g) Calculate the radius of the free fermion electron Fermi sphere (circle in 2D) in cm^{-1} if the metal had valency 4. (5 points)

We need to repeat the calculation done (d) but now $N = 4$. This means that the radius of the circle is double and thus, $k_F = 17.72 \times 10^7 \text{ cm}^{-1}$.

- h) Draw this sphere to scale on your drawing of the Brillouin zones. (5 points)

- i) Indicate the occupation of the first, second, and third Brillouin zones if the metal had valency 4, i.e. say if the zones are occupied or empty. (5 points)

Now the FBZ is filled while the second and third are partially occupied and even a bit of the fourth zone is occupied.

Problem 2: Consider a two-dimensional square lattice with lattice constant a .

- a) Provide a set of primitive vectors in reciprocal space. (5 points)

The primitive vectors are

$$\mathbf{b}_1 = \frac{2\pi}{a}(1, 0); \mathbf{b}_2 = \frac{2\pi}{a}(0, 1). \quad (5)$$

b) For the points in reciprocal space listed below identify their location in terms of the primitive vectors and calculate the value of the kinetic energy of a free electron at

i) a corner of the first Brillouin zone (Hint: how many corners does the Brillouin zone have? Will your answer depend on what corner you choose?); (5 points)

The FBZ is a square centered at the origin that runs from $-\pi/a$ to π/a along k_x and from $-\pi/a$ to π/a along k_y . Thus, one corner is at point $\mathbf{k}_M = (\pi/a, \pi/a)$. At this point the kinetic energy of a free electron is given by

$$E_M = \frac{\hbar^2 k_M^2}{2m} = \frac{\hbar^2 2\pi^2}{2ma^2} = \frac{\hbar^2 \pi^2}{ma^2}. \quad (6)$$

ii) a midpoint of the boundary of the first Brillouin zone (Hint: think how many boundaries (sides) the FBZ has and if your answer will depend on the boundary you chose) . (5 points)

One of the boundary middle points is X at $\mathbf{k}_X = (\pi/a, 0)$. At this point the kinetic energy of a free electron is given by

$$E_X = \frac{\hbar^2 k_X^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2}. \quad (7)$$

Notice that $\mathbf{k}_X = \mathbf{k}_1$ required in part c-iii.

iii) Provide the ratio of the energy obtained in (i) with the energy obtained in (ii). (5 points)

The ratio R between the two energies is given by

$$R = \frac{E_M}{E_X} = 2. \quad (8)$$

c) The crystal potential of the corresponding material is

$$V(x, y) = -2V_0(\cos \frac{2\pi x}{a} + \cos \frac{2\pi y}{a}),$$

where V_0 is a constant.

i) How many values of K are needed to describe the potential? (5 points)

Notice that we can write the potential as:

$$V(x, y) = -V_0(e^{\frac{2i\pi x}{a}} + e^{\frac{-2i\pi x}{a}} + e^{\frac{2i\pi y}{a}} + e^{\frac{-2i\pi y}{a}}) = -V_0(e^{ib_1 \cdot x} + e^{-ib_1 \cdot x} + e^{ib_2 \cdot y} + e^{-ib_2 \cdot y}). \quad (9)$$

This means that we need only 4 reciprocal lattice vectors to expand the potential. Those are: \mathbf{b}_1 , \mathbf{b}_2 , $-\mathbf{b}_1$, and $-\mathbf{b}_2$.

ii) Label each of the needed reciprocal lattice vectors K_i with $i = 1, \dots, R$ where R is the number of K needed and express each K_i in terms of the vectors of the primitive basis that you found in (a). (5 points)

$\mathbf{K}_1 = \mathbf{b}_1$, $\mathbf{K}_2 = \mathbf{b}_2$, $\mathbf{K}_3 = -\mathbf{b}_1$, and $\mathbf{K}_4 = -\mathbf{b}_2$.

iii) At the midpoint of the first Brillouin zone boundary whose momentum \mathbf{k}_1 you identified in b-ii, the electronic wave function $\Psi(\mathbf{k}_1)$ will couple strongly to another component of Ψ , $\Psi(\mathbf{k}_2)$. What is \mathbf{k}_2 ? (5 points)

We notice that at $\mathbf{k}_2 = (-\pi/a, 0)$ the energy is the same than at $\mathbf{k}_1 = (\pi/a, 0)$. Thus, these are the two components of Ψ that will get strongly coupled.

iv) What is the value of \mathbf{K} that one must include when doing perturbation theory to find $\Psi(\mathbf{k}_1)$ and $\Psi(\mathbf{k}_2)$ to first order in V_0 ? (5 points)

Since $\mathbf{k}_2 = (-\pi/a, 0) = \mathbf{k}_1 - \mathbf{K}_1$, this is the K that we need to include in the perturbative calculation.

v) Write down the Schrödinger equation in the subspace involving $\Psi(\mathbf{k}_1)$ and $\Psi(\mathbf{k}_2)$. (5 points)

$$\frac{\hbar^2 k_1^2}{2m} \Psi(\mathbf{k}_1) + U_{\mathbf{k}_1 - \mathbf{k}_2} \Psi(\mathbf{k}_2) = \epsilon \Psi(\mathbf{k}_1) \quad (10)$$

$$\frac{\hbar^2 k_2^2}{2m} \Psi(\mathbf{k}_2) + U_{\mathbf{k}_2 - \mathbf{k}_1} \Psi(\mathbf{k}_1) = \epsilon \Psi(\mathbf{k}_2) \quad (11)$$

Notice that $U_{\mathbf{K}_1} = U_{-\mathbf{K}_1} = -V_0$ and $\frac{\hbar^2 k_1^2}{2m} = \epsilon_{\mathbf{k}_1} = \epsilon_{\mathbf{k}_2} = \frac{\hbar^2 k_2^2}{2m}$.

vi) Solve the 2x2 system of equations and find the two allowed energies at Bloch index \mathbf{k}_1 . (5 points)

The determinant that we need to solve is:

$$\begin{vmatrix} \epsilon_{\mathbf{k}_1} - \epsilon & U_K \\ U_{-K} & \epsilon_{\mathbf{k}_2} - \epsilon \end{vmatrix} = 0. \quad (12)$$

The characteristic equation is

$$(\epsilon_{\mathbf{k}_1} - \epsilon)^2 - V_0^2 = 0. \quad (13)$$

The solutions are:

$$\epsilon_{\pm} = \frac{\hbar^2 \pi^2}{2ma^2} \pm V_0. \quad (14)$$

vii) Provide the value of the energy gap at \mathbf{k}_1 . (5 points)

The energy gap is given by $\epsilon_+ - \epsilon_- = V_0 - (-V_0) = 2V_0$.