Second Midterm Exam

P555

March 26, 2020

SHOW ALL YOUR WORK TO GET FULL CREDIT!

Submit a pdf file with your work not later that March 26 at 8PM.

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

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

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

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

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

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

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

g) Calculate the radius, at $T = 0$, of the free fermion electron Fermi sphere (circle in 2D) in cm^{-1} if the metal had valency 4. (5 points)

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)

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

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

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)

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)

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

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)

ii) Label each of the needed reciprocal lattice vectors K_i with $i = 1, ..., R$ 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)

iii) At the midpoint of the first Brouillin 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)

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)

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

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

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