

I. PROBLEM SESSION 11

A. Problem 11.1

(Exercise 7.2 Kittel)

Free electron energies in the reduced zone scheme:

Consider the free electron energy bands of an fcc crystal lattice in the approximation of an empty lattice, but in the reduced zone scheme (in which all \vec{k} 's are transformed to lie in the first Brillouin zone). Plot roughly in the $[1, 1, 1]$ direction the energies of all bands up to six times the lowest band energy at the zone boundary at $\vec{k} = (2\pi/a)(1/2, 1/2, 1/2)$. Let this be the unit of energy. This problem shows why band edges need not necessarily be at the zone center. Several of the degeneracies (band crossings) will be removed when the crystal potential is taken into account.

B. Problem 11.2

(Exercise 7.6 Kittel)

Band gap for a square lattice: Consider a square lattice in two dimensions with the crystal potential

$$U(x, y) = -4U \cos\left(\frac{2\pi x}{a}\right) \cos\left(\frac{2\pi y}{a}\right). \quad (1)$$

Apply the central equation to find approximately the energy gap at the corner point $(\pi/a, \pi/a)$ of the Brillouin zone. It will suffice to solve a 2×2 determinantal equation.