

1. (ISSP 7.1).

(a) At the center of a face,  $\vec{k} = (\pi/a, 0)$  and so

$$E_{face} = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2}{2ma^2}$$

At the corner,  $\vec{k} = (\pi/a, \pi/a)$  and so  $k = \sqrt{2}(\pi/a)$ , giving

$$E_{corner} = \frac{\hbar^2 k^2}{2m} = 2 \frac{\hbar^2 \pi^2}{2ma^2}$$

Therefore the energy is twice as high at the corner than it is at the face.

(b) At the corner of the 3D lattice,  $\vec{k} = (\pi/a, \pi/a, \pi/a)$  and so  $k = \sqrt{3}(\pi/a)$ , giving

$$E_{corner} = \frac{\hbar^2 k^2}{2m} = 3 \frac{\hbar^2 \pi^2}{2ma^2}$$

(c) Recall that there are  $2N$  states in every band. Therefore you might expect that the electrons in the divalent element would fill up the lowest band and it would be a band insulator. However, if the gap at  $\vec{k} = (\pi/a, 0, 0)$  to the next highest band is smaller than  $3 \frac{\hbar^2 \pi^2}{2ma^2} - \frac{\hbar^2 \pi^2}{2ma^2} = 2 \frac{\hbar^2 \pi^2}{2ma^2}$ , then this band will be partially occupied, the lowest band will be partially empty and the element will be a metal.

2. (ISSP 7.2).

The free electron bands come from translating the free electron dispersion back into the Brillouin zone. Let  $\vec{k}$  be a wavevector in the first Brillouin zone, and let's denote the different bands using the index  $n$ . Then for each  $n$ , the dispersion  $E_n(\vec{k}) = (\hbar^2/2m)(\vec{k} + \vec{G})^2$  for some reciprocal lattice vector  $\vec{G}$ .

The reciprocal lattice vectors for an fcc lattice can be written as  $\vec{G} = h\vec{b}_1 + l\vec{b}_2 + m\vec{b}_3$ , where  $\vec{b}_i$  are given in equation (36) on page 38 of ISSP. Then, letting  $\vec{k} = \alpha(2\pi/a)(1/2, 1/2, 1/2)$ , where  $\alpha \in [0, 1]$ ,

$$(\vec{k} + \vec{G})^2 = \left(\frac{2\pi}{a}\right)^2 \left[ \left(\frac{\alpha}{2} - h + l + m\right)^2 + \left(\frac{\alpha}{2} + h - l + m\right)^2 + \left(\frac{\alpha}{2} + h + l - m\right)^2 \right]$$

So each choice of  $h, l$  and  $m$  give a different band, and the dispersion of that band in the [111] direction is

$$\begin{aligned} E_{hlm}(k) &= \frac{\hbar^2}{2m} \left(\frac{2\pi}{a}\right)^2 \left[ \left(\frac{\alpha}{2} - h + l + m\right)^2 + \left(\frac{\alpha}{2} + h - l + m\right)^2 + \left(\frac{\alpha}{2} + h + l - m\right)^2 \right] \\ &= \frac{\hbar^2}{2m} \left(\frac{2\pi}{a}\right)^2 \left[ \frac{3}{4}\alpha^2 + \alpha(h + l + m) + (h - l)^2 + (h - m)^2 + (l - m)^2 + h^2 + l^2 + m^2 \right] \end{aligned}$$

The dispersion is shown in figure 1.

3. (ISSP 7.3).

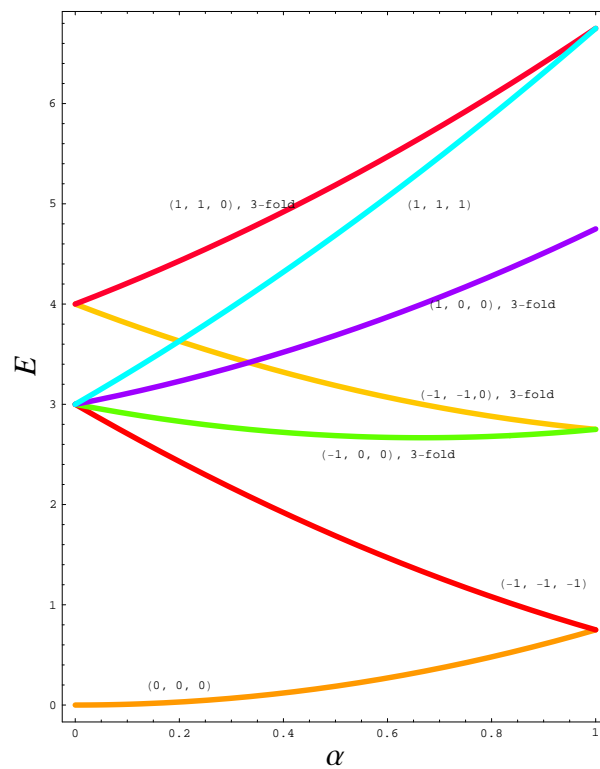


Figure 1: Q2, the free electron bands for the fcc lattice in the  $[111]$  direction. The energy is measured in units of  $(\hbar^2/2m)(2\pi/a)^2$ . The triplet of numbers indicates the values of  $(h, l, m)$  associated with the branch. If the degeneracy of a band is different from 1, I've indicated it in the figure. For instance, the bands corresponding to  $(h, l, m) = (1, 0, 0), (0, 1, 0), (0, 0, 1)$  all lie on top of each other.

(a) Equation 21b on page 169 of ISSP reads, when  $k = 0$ ,

$$P \frac{\sin Ka}{Ka} + \cos Ka = 1$$

When  $P = 0$ ,  $K = 0$ , and so if  $P$  is small we can expect  $Ka$  to be small. Then

$$P \left( 1 - \frac{(Ka)^2}{6} \right) + 1 - \frac{(Ka)^2}{2} = 1 \Rightarrow (Ka)^2 = \frac{6P}{P+3} \simeq 2P$$

The energy is therefore

$$E = \frac{\hbar^2}{2ma^2} (Ka)^2 = \frac{\hbar^2 P}{ma^2}$$

(b) At  $k = \pi/a$ ,

$$P \frac{\sin Ka}{Ka} + \cos Ka = -1$$

Consider  $Ka = \pi + \Delta$ . Then for  $P = 0$ ,  $\Delta = 0$  and so we can expect  $\Delta$  to be small also. Then

$$-P \frac{\sin \Delta}{\pi + \Delta} - \cos \Delta = -1$$

and so

$$P \left( -\frac{\Delta}{\pi} + \frac{\Delta^2}{\pi^2} \right) - 1 + \frac{\Delta^2}{2} = -1 \Rightarrow \Delta^2 \left( \frac{1}{2} + \frac{P}{\pi^2} \right) - \frac{P}{\pi} \Delta = 0$$

Therefore the two smallest solutions are  $\Delta = 0$  and

$$\Delta = \frac{P/\pi}{P/\pi^2 + 1/2} \simeq \frac{2P}{\pi}$$

Therefore, to first order in  $P$ , the energy gap is

$$E_g = \frac{\hbar^2}{2ma^2} \left( \pi + \frac{2P}{\pi} \right)^2 - \frac{\hbar^2}{2ma^2} (\pi + 0)^2 \simeq \frac{\hbar^2 4P}{2ma^2} = \frac{2\hbar^2 P}{ma^2}$$

4. (ISSP 7.6). The potential can be rewritten as

$$U(\vec{r}) = -U \left( e^{i(\frac{2\pi}{a}, \frac{2\pi}{a}) \cdot \vec{r}} + e^{i(\frac{-2\pi}{a}, \frac{2\pi}{a}) \cdot \vec{r}} + e^{i(\frac{2\pi}{a}, \frac{-2\pi}{a}) \cdot \vec{r}} + e^{i(\frac{-2\pi}{a}, \frac{-2\pi}{a}) \cdot \vec{r}} \right)$$

Therefore the degenerate states at  $\vec{k} = (\pi/a, \pi/a)$  and  $(-\pi/a, -\pi/a)$  are coupled by  $\vec{G} = (-2\pi/a, -2\pi/a)$ . (The other  $G$ -vectors couple  $(\pi/a, \pi/a)$  to states that are higher in energy.) Applying degenerate perturbation theory as on page 178 of ISSP gives

$$\begin{vmatrix} \frac{\hbar^2 k^2}{2m} - E & U \\ U & \frac{\hbar^2 k^2}{2m} - E \end{vmatrix} = 0$$

and so

$$E = \frac{\hbar^2 k^2}{2m} \pm U$$

giving a gap of  $2U$ .