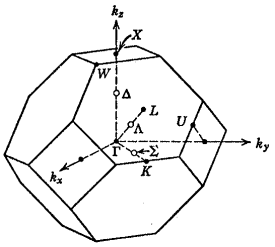
CHAPTER 7

1a. The wavevector at the corner is longer than the wavevector at the midpoint of a side by the factor √2. As $\varepsilon \propto k^2$ for a free electron, the energy is higher by $(\sqrt{2})^2 = 2$. b. In three dimensions the energy at a corner is higher by $(\sqrt{3})^2$ than at the midpoint of a face. c. Unless the band gap at the midpoint of a face is larger than the kinetic energy difference between this point and a corner, the electrons will spill over into the second zone in preference to filling up the corner states in the first zone. Divalent elements under these conditions will be metals and not insulators.

2. $\varepsilon = \hbar^2 k^2/2m$, where the free electron wavevector k may be written as the sum of a vector K in the reduced zone and of a reciprocal lattice vector G. We are interested in K along the [111] direction: from



Chap. 2, K = (2 π / a) (1,1,1) u, with $0 < u < \frac{1}{2}$, will lie in the reduced zone. The G´s of the reciprocal lattice are given by $G = (2\pi/a)[(h-k+\ell)\hat{x} + (h+k-\ell)\hat{y} + (-h+k+\ell)\hat{z}]$, where h, k, ℓ are any integers. Then $\varepsilon = (\hbar^2/2m)(2\pi/a)^2[(u+h-k+\ell)^2 + (u+h+k-\ell)^2 + (u-h+k+\ell)^2]$. We now have to consider all combinations of indices h, k, ℓ for which the term in brackets is smaller than $6[3(1/2)^2]$ or 9/2. These indices are (000); $(\bar{1}\bar{1}\bar{1})$; $(\bar{1}00)$, $(0\bar{1}0)$, and $(00\bar{1})$; (100), (010), and (001); (111); $(\bar{1}\bar{1}0)$, $(\bar{1}0\bar{1})$, and $(0\bar{1}\bar{1})$; (110), (101), and (011).

3. (a) At k = 0 the determinantal equation is (P/Ka) sin Ka + cos Ka = 1. In the limit of small positive P this equation will have a solution only when $Ka \ll 1$. Expand the sine and cosine to obtain in lowest order $P \simeq \frac{1}{2}(Ka)^2$. The energy is $\varepsilon = \hbar^2 K^2/2m \simeq \hbar^2 P/ma^2$. (b) At k = π/a the determinantal equation is (P/Ka) sin Ka + cos Ka = –1. In the same limit this equation has solutions Ka = π + δ, where $\delta \ll 1$. We expand to obtain $(P/\pi)(-\delta) + \left(-1 + \frac{1}{2}\delta^2\right) = -1$, which has the solution δ = 0 and δ = 2P/π. The energy gap is $E_g = (\hbar^2/2ma^2)(2\pi\delta) \simeq (\hbar^2/2ma^2)(4P)$.

4. (a) There are two atoms in the basis, and we label them a and b. Then the crystal potential may be written as $U = U_1 + U_2 = U_1(\underset{\sim}{r}) + U_1\left(x + \frac{1}{4}a,\, y + \frac{1}{4}a,\, z + \frac{1}{4}a\right)$ and the Fourier transform has components $U_{\underset{\sim}{G}} = U_{1\underset{\sim}{G}} + U_{2\underset{\sim}{G}} = U_{1\underset{\sim}{G}}\left(1 + e^{i(G_x+G_y+G_z)\frac{1}{4}a}\right)$. If $\underset{\sim}{G} = 2A\hat{\underset{\sim}{x}}$, then the exponential is $e^{i\frac{1}{2}Aa} = e^{i\pi} = -1$, and $U_{\underset{\sim}{G}=2A} = 0$, so that this Fourier component vanishes. Note that the quantity in parentheses above is just the structure factor of the basis. (b) This follows directly from (44) with U set equal to zero. In a higher order approximation we would go back to Eq. (31) where any non-vanishing $U_{\underset{\sim}{G}}$ enters.

5. Let $k = K + iH$; $\lambda_{\pm 1} = \frac{\hbar^2}{2m}\left[\left(\frac{1}{2}G\right)^2 \pm iGH - H^2\right]$.

The secular equation (46) is now

$$\begin{vmatrix} \lambda_1 - \varepsilon & U \\ U & \lambda_{-1} - \varepsilon \end{vmatrix} = 0,$$

and for $H << G$ we have, with $\sigma = \varepsilon - \frac{\hbar^2}{2m}\left(\frac{1}{2}G\right)^2$,

$$\left(\sigma + iGH \cdot \frac{\hbar^2}{2m}\right)\left(\sigma - iGH\,\frac{\hbar^2}{2m}\right) = U_1^{\,2};$$

$$\sigma^2 - \left(\frac{\hbar^2}{2m}GH\right)^2 = U_1^{\,2};$$

$$\therefore \frac{\hbar^2}{2m}H^2 = \frac{U_1^{\,2} - \sigma}{\frac{\hbar^2}{2m}G^2}.$$

6. $U(x,y) = -U[e^{i\,(2\pi/a)\,(x+y)}$ + other sign combinations of $\pm x \pm y]$. The potential energy contains the four reciprocal lattice vectors $(2\,\pi/a)\,(\pm 1; \pm 1)$. At the zone corner the wave function $e^{i(\pi/a)\,(x+y)}$ is mixed with $e^{-i\,(\pi/a)\,(x+y)}$. The central equations are

$$(\lambda - \varepsilon)C\left[\frac{\pi}{a}; \frac{\pi}{a}\right] - UC\left[-\frac{\pi}{a}; -\frac{\pi}{a}\right] = 0\ ;$$

$$(\lambda - \varepsilon)C\left[-\frac{\pi}{a}; -\frac{\pi}{a}\right] - UC\left[\frac{\pi}{a}; \frac{\pi}{a}\right] = 0\ ,$$

where $\lambda = 2\left(\hbar^2/2m\right)\left(\pi/a\right)^2$. The gap is 2U.