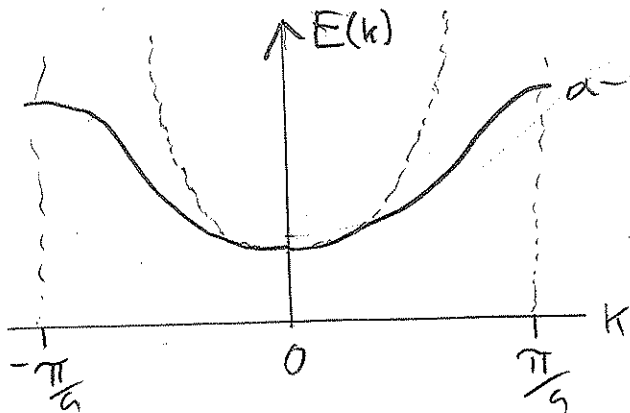


(HWrk see Fri. notes 3, read 15.6 in McIntyre)

Day 12 Recall the ground state of valence band

energies are  $E(k) = \alpha + 2\beta \cos ka$

$\approx \alpha + 2\beta(1 - \frac{1}{2}(ka)^2)$ , for small  $ka$



Near  $k=0$  the band looks parabolic, which reminds us of the free-electron dispersion,  $E(k) = \frac{\hbar^2 k^2}{2m_e}$

Specifically for,  $E(k) - E(k=0) \approx \beta(ka)^2$

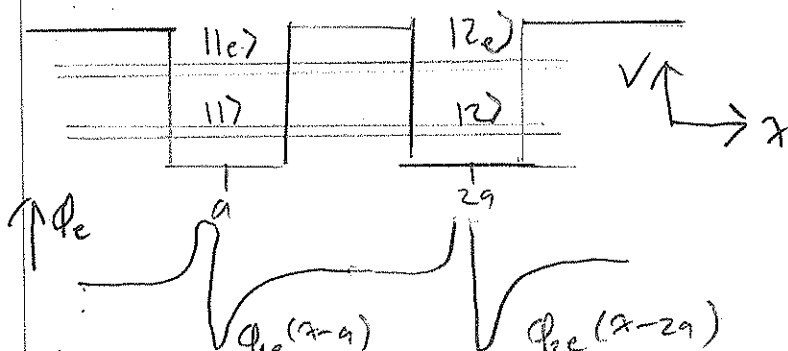
$\approx \frac{\hbar^2 k^2}{2m^*}$

where  $m^*$  is the effective mass,  $m^* \equiv \frac{\hbar^2}{2|\beta|a^2}$

rigorously, the effective mass is the free-electron mass "dressed" by the potential field of the crystal,

in general,  $m^* \equiv \hbar^2 \left[ \frac{d^2 E}{dk^2} \Big|_{k=k_0} \right]^{-1}$

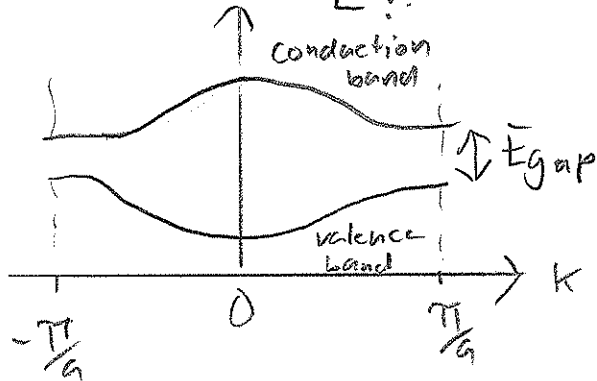
What about the excited state w.f.  $|1e\rangle, |2e\rangle, \dots, |Ne\rangle$  and the conduction band?



excited state w.f. is odd,  $\Phi_e(-x) = -\Phi_e(x)$   
 $\Rightarrow \beta_e = \langle 2e | \hat{H} | 1e \rangle$   
 $= \langle 2e | \hat{V}(x-a) | 1e \rangle + \langle 2e | \hat{V}(x-2a) | 1e \rangle > 0$

Hence,  $\beta_c > 0$  (recall  $\beta < 0$ )

Thus,  $\hat{H} = \begin{bmatrix} \alpha_e & \beta_c & 0 & \dots \\ \beta_c & \alpha_c & \beta_c & \dots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$  or  $E(k) = \alpha_e + 2\beta_c \cos ka$



Band-gap: min energy spacing between bands.

$$E_{gap} \cong (\alpha_e + 2\beta) - (\alpha - 2\beta)$$

Fermi Energy: the maximum occupied energy at  $T=0K$

If  $E_F$  is in the band gap at  $T=0K$ , the material

is a semiconductor or insulator. If  $E_F$  lies within a band it is a metal

Semiconductors are further classified as direct or indirect

it is a direct gap if the lowest point in the conduction band occurs at the same  $k$ -value as the highest energy in the valence band,

Band-width: the difference in the maximum and minimum energy allowed in each band.

e.g.  $E_w = E(0) - E(\pi/a) = 4\beta$  for  $q$ -well valence band  
 $4\beta_c$  for conduction band