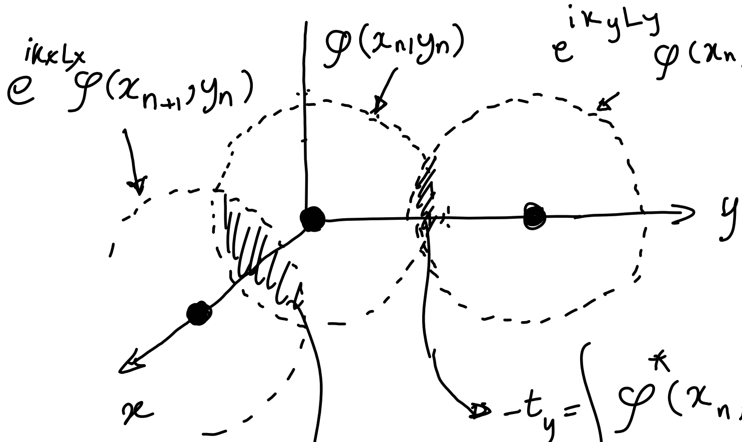
Tight Bonding approximation (cont.)

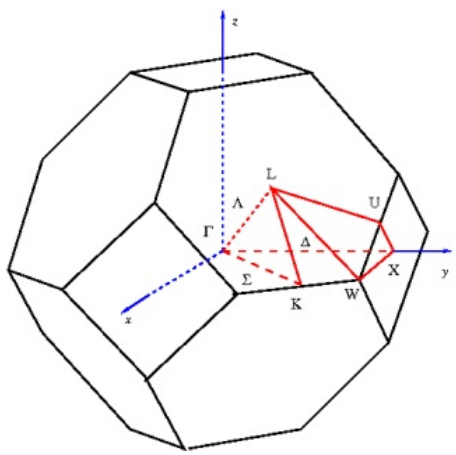


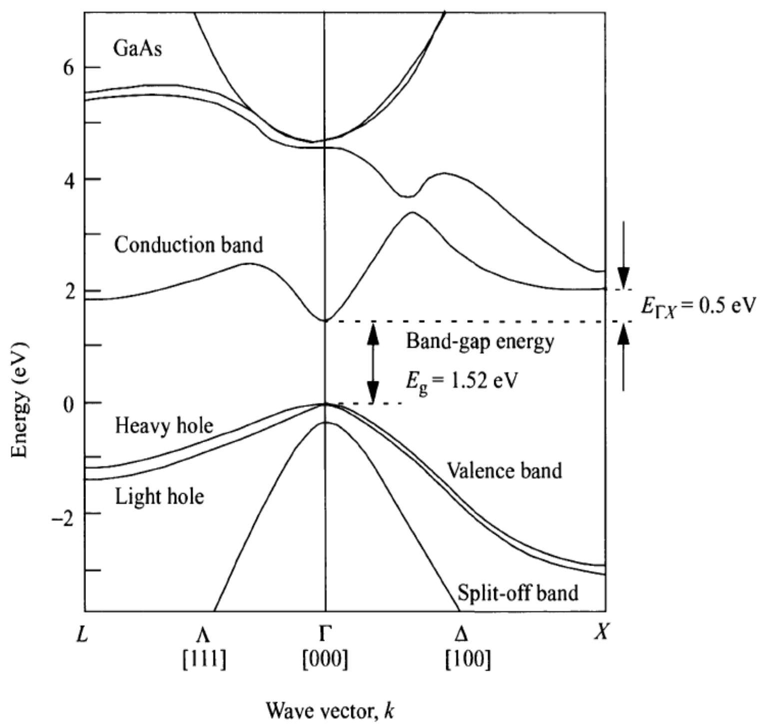
Hopping integrals:

wannier function

$$-t_y = \int \varphi^*(x_n,y_n)\hat{H}\varphi(x_n,y_{n\pm1}) \Rightarrow E_y(k)$$

$$-t_x = \int \varphi^*(x_n,y_n)\hat{H}\varphi(x_{n\pm1},y_n) \Rightarrow E_x(k)$$





Crystal momentum

$E = \hbar\omega$

For free electron: $E = \frac{\hbar^2 k^2}{2m}$

For electron in crystall: $E(k)$, $\omega(k)$

Group velocity of electron wave packet: $v_g = \frac{\partial \omega}{\partial k}$

Effective mass

$$m \longrightarrow m(k)$$

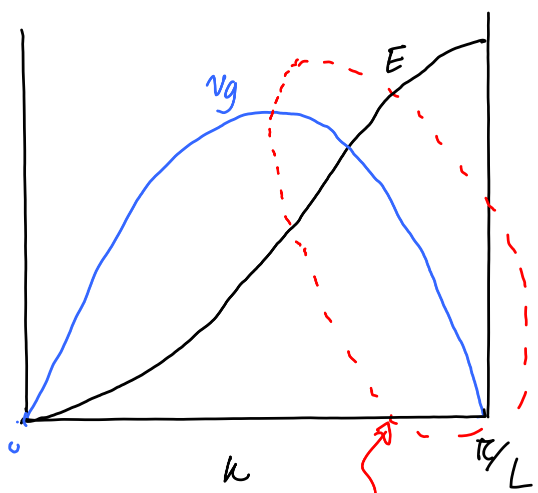
$$m(k) = \frac{\hbar}{\frac{\partial^2 \omega}{\partial k^2}} = m_{eff}(k)\, m_e$$

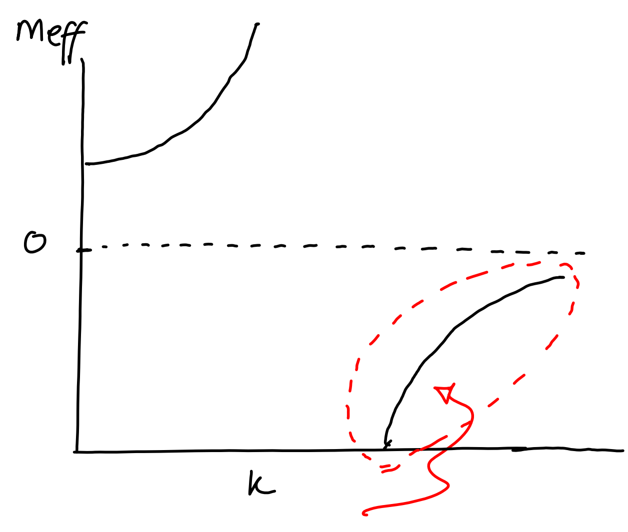
Let's check with the dispersion relation derived in our 1D tight bonding model :

$$E(k) = \frac{E_b}{2}(1 - \cos kL) = E_b \sin^2\left(\frac{kL}{2}\right)$$

$$v_g = \frac{\partial \omega}{\partial k} = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \frac{E_b L}{2\hbar} \sin(kL)$$

$$m^*(k) = \frac{\hbar}{\partial^2\omega/\partial k^2} = \frac{2\hbar^2}{E_b L^2 \cos(kL)}$$





Negative effective mass

Check v_g : velocity v_g is decreased as the wave vector k is increased.