

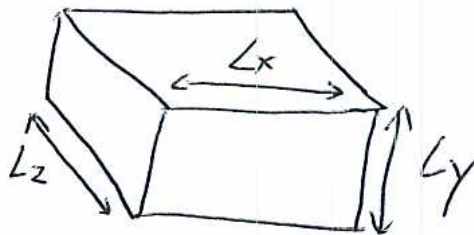
## (b) Density of states

we want to know the Dos in energy  $g(E) dE$ ;  
 however it is much easier to derive first the  
 Dos in  $k$ -space  $g(k) dk$ .

Since  $\boxed{g(E) dE = g(k) dk}$   
 if we get  $g(k)$  and  $E(k) \xrightarrow{\text{we obtain}}$   $g(E)$ .  
 $\uparrow$   
 dispersion  
 relation

### In $k$ -space

we consider a crystal with macroscopic  
 dimension



we know that  $\psi(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{\vec{k}}(\vec{r})$  and  $u_{\vec{k}}(\vec{r} + \vec{T}) = u_{\vec{k}}(\vec{r})$ ,  
 for each unit cells.

How can we choose the boundary conditions at the edge of the solid?

⇒ rather than vanishing B.C ( $\Psi=0$ ), we make use of periodic B.C [Born-Van Karman] for allowing traveling-wave.

At the edges  $\boxed{\Psi(\vec{r}+L) = \Psi(\vec{r})}^*$

$$\Psi(\vec{r}+\vec{L}) = e^{i(\vec{k}\vec{r}+\vec{L})} u_{\vec{k}}(\vec{r}+\vec{L})$$

$$\Psi(\vec{r}+\vec{L}) = e^{i\vec{k}\vec{r}} u_{\vec{k}}(\vec{r}) e^{i\vec{k}\vec{L}}$$

$$\Psi(\vec{r}+\vec{L}) = \Psi(\vec{r}) e^{i\vec{k}\vec{L}} \xrightarrow{\text{with } (*)} e^{i\vec{k}\vec{L}} = 1$$

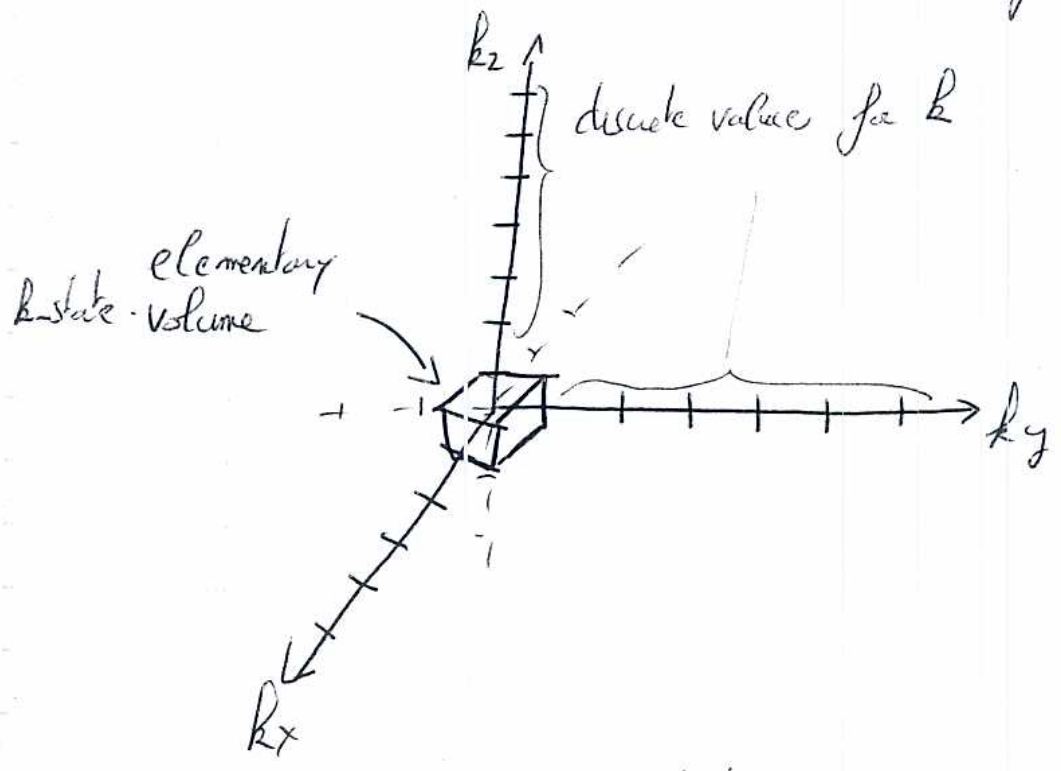
true if  $k_x = m_x \frac{2\pi}{L_x}$  ;  $k_y = m_y \frac{2\pi}{L_y}$  ;  $k_z = m_z \frac{2\pi}{L_z}$

⇒ discrete k values

$$m_x, m_y, m_z \in \mathbb{Z} (= \dots -2, -1, 0, 1, 2, \dots)$$

⇒ 2 directions of propagation.

the elementary volume in  $k$ -space is  $\frac{(2\pi)^3}{L_x L_y L_z}$



the number of  $k$  states that we obtain in a volume  $d\vec{k}$  (or  $d^D k$   $D=1,2,3$ ) is  $\left( \frac{d^D k}{\frac{(2\pi)^D}{L^D}} \right)$

it comes 
$$g(k) d^D k = 2 \frac{L^D}{(2\pi)^D} d^D k \quad (2 \text{ for spin})$$

$L^D$  is the volume of the crystal  $\left( \begin{array}{l} L^D = L \text{ in } 1D \\ L^D = S \text{ in } 2D \\ L^D = V \text{ in } 3D \end{array} \right)$

$\Rightarrow g(k)$  is per unit of volume

in 3D  $d^3k = 4\pi k^2 dk$  (elementary volume between 2 spheres)

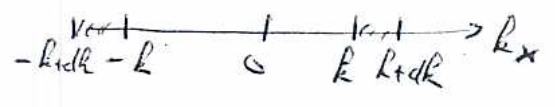
$$\Rightarrow \boxed{g(k) dk = \frac{2 \cdot 4\pi k^2 dk}{(2\pi)^3}}$$

in 2D  $d^2k = 2\pi k dk$  (elementary volume between two circles)

$$\Rightarrow \boxed{g(k) dk = \frac{2 \cdot 2\pi k dk}{(2\pi)^2}}$$

in 1D  $dk = 2 dk$  (2 directions of propagation)

$$\Rightarrow \boxed{g(k) dk = \frac{2 \cdot 2 dk}{(2\pi)}}$$



In order to obtain  $g(E)$ ; one now needs to know  $E(k)$ . since

$$\boxed{g(E) = g(k) \left( \frac{dE}{dk} \right)^{-1}}$$

$g(k)$  per unit of energy and volume



\* For the  $e^-$  in the effective mass approach

$$E(k) = \frac{\hbar^2 k^2}{2m_n^*} + E_c \Rightarrow \frac{dE}{dk}$$

$$\Rightarrow g_c(\bar{E}) dE = \frac{m_n^* \sqrt{2m_n^* (E - E_c)}}{\pi^2 \hbar^3} dE \quad E \geq E_c \quad (2.6a)$$

for holes  $E(k) = -\frac{\hbar^2 k^2}{2m_p^*} + E_v \Rightarrow \frac{dE}{dk}$

$$g_v(E) dE = \frac{m_p^* \sqrt{2m_p^* (E_v - E)}}{\pi^2 \hbar^3} dE \quad E \leq E_v \quad (2.6b)$$

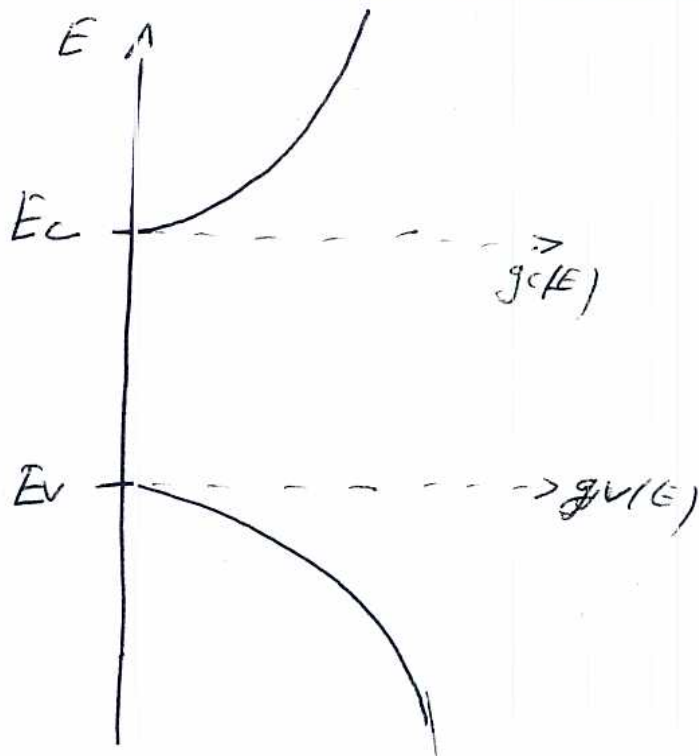


Fig 1 \* gives the different DOS obtained for 1D, 2D and 3D systems.

Fig 2 \* In general, for  $e^-$  in periodic crystal, the dispersion relation  $E(k)$  does not have a simple analytical form and then  $g(E)$

Figure 1

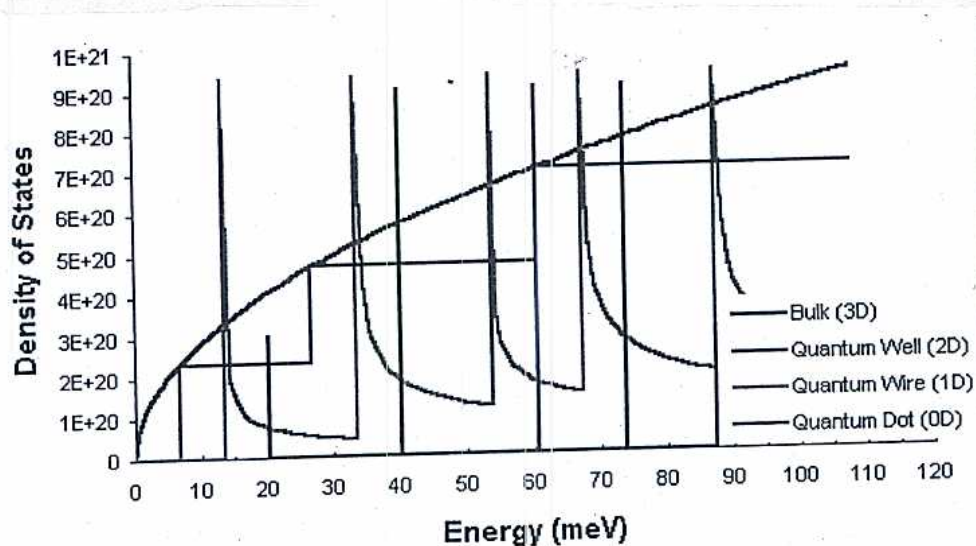


Figure 2

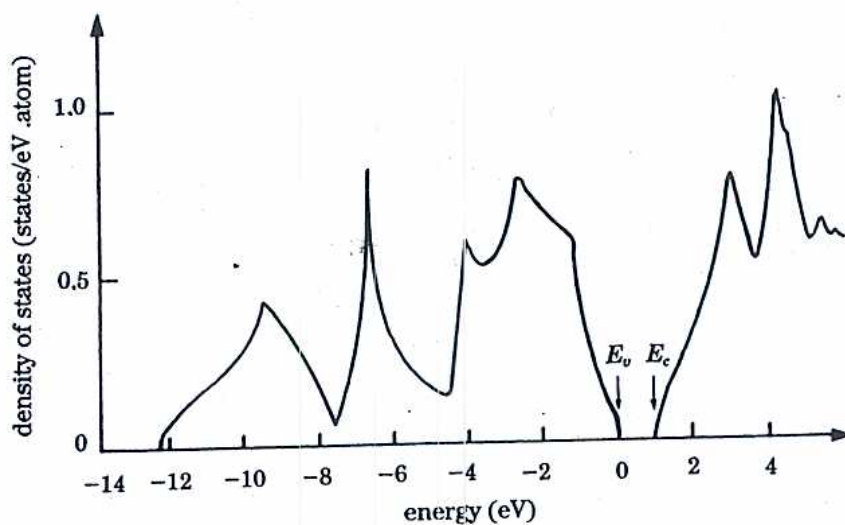


Fig. 2.5. Density of states of the valence and conduction bands of silicon, calculated by J.R. Chelikowsky and M.L. Cohen, Physical Review B 14, 556 (1976). The energy origin is at the maximum  $E_v$  of the valence band. In the neighborhood of  $E_v$ , the maximum of the valence band, and  $E_c$ , the minimum of the conduction band, the density of states varies parabolically with energy.