

Primer on Semiconductors

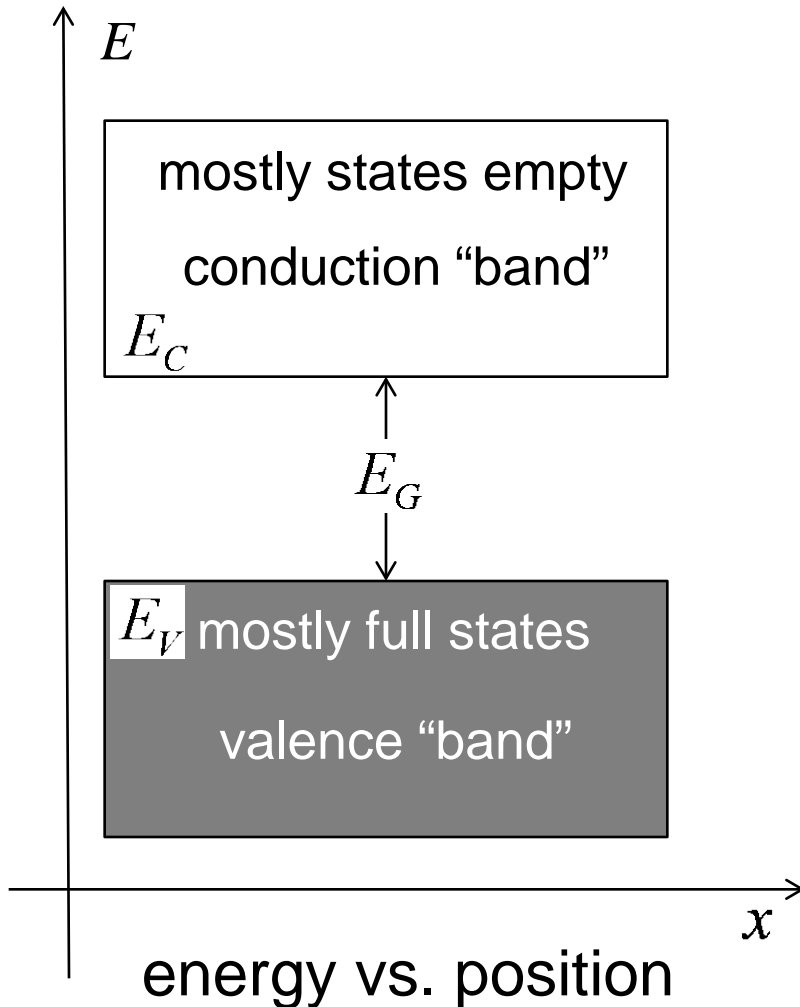
Unit 2: Quantum Mechanics

Lecture 2.5: Density of states

Mark Lundstrom

lundstro@purdue.edu
Electrical and Computer Engineering
Purdue University
West Lafayette, Indiana USA

Conduction and valence bands



It will be important for us to know how the states are distributed in energy within the conduction and valence bands.

Most of the empty states (the holes) in the valence band are very near E_V .

Most of the filled states (the electrons) in the conduction band are very near E_C .

Density of states

The number of states between E and $E + dE$ is $D(E)dE$, where $D(E)$ is the “density of states” (DOS).

In this lecture, we will calculate the DOS. This calculation is greatly simplified because only the region near the band edges are important, and in that region, the bands are nearly parabolic:

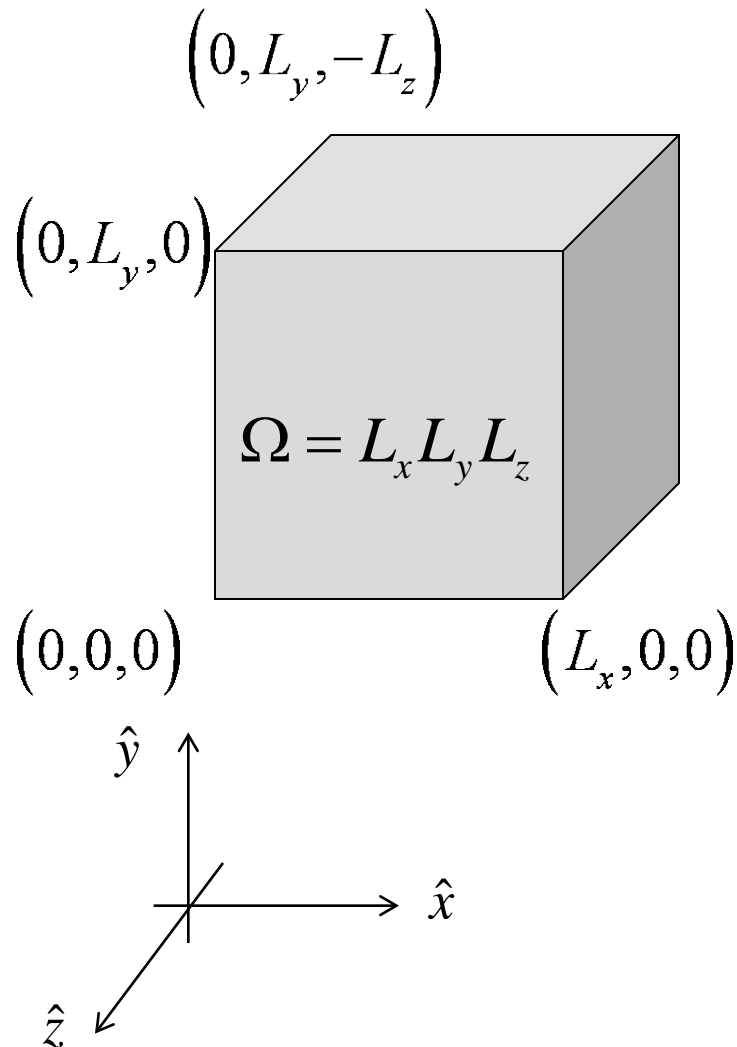
$$E(k) = E_V - \frac{\hbar^2 k^2}{2m_p^*}$$

valence
band

$$E(k) = E_C + \frac{\hbar^2 k^2}{2m_n^*}$$

conduction band

States in a finite volume of semiconductor



Finite volume, Ω
(***part of an infinite volume***)

Finite number of states

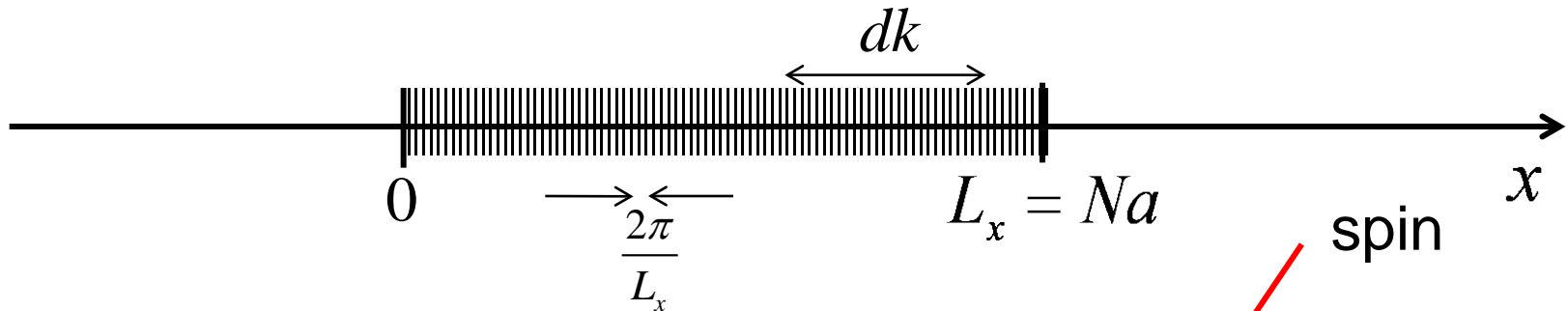
Periodic boundary conditions:

$$\psi(0,0,0) = \psi(L_x,0,0)$$

$$\psi(0,0,0) = \psi(0,L_y,0)$$

$$\psi(0,0,0) = \psi(0,0,L_z)$$

x-direction



$$\psi(x) = u_k(x)e^{ik_x x}$$

$$\psi(0) = \psi(L_x) \rightarrow e^{ik_x L_x} = 1$$

$$k_x L_x = 2\pi j \quad j = 1, 2, 3, \dots$$

$$k_x = \frac{2\pi}{L_x} j$$

$$\# \text{ of states} = \frac{dk_x}{(2\pi/L_x)} \times 2 = N_k dk$$

$$N_k = \frac{L_x}{\pi} = \text{density of states in } k\text{-space}$$

$$L_x = Na \quad k_x = \frac{2\pi}{a} \frac{j}{N} \quad j_{\max} = N$$

“Brillouin zone” $0 < k < \frac{2\pi}{a}$ $k_{\max} = \frac{2\pi}{a}$

Density-of-states in k-space

1D:

$$N_k = 2 \times \left(\frac{L}{2\pi} \right) = \frac{L}{\pi} \quad dk$$

2D:

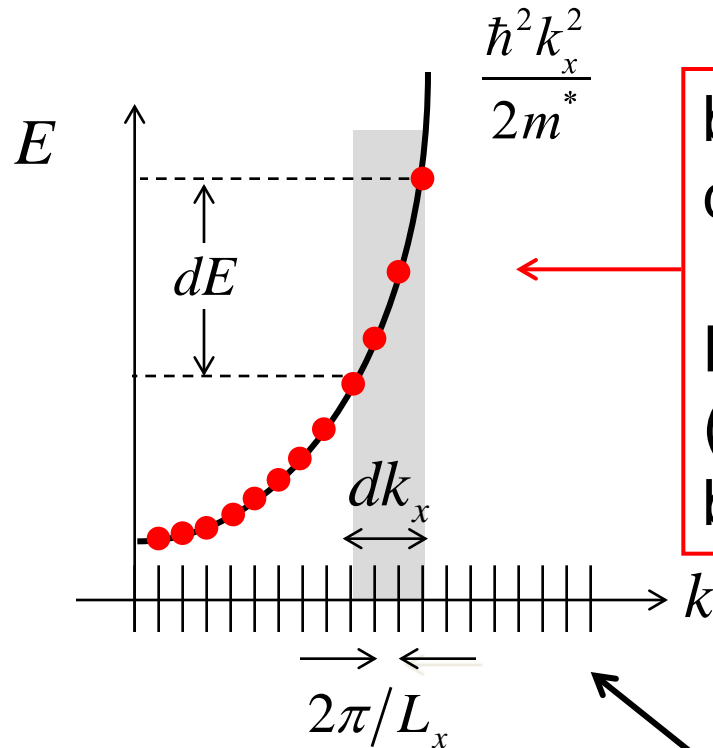
$$N_k = 2 \times \left(\frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} \quad dk_x dk_y$$

independent of $E(k)$

3D:

$$N_k = 2 \times \left(\frac{\Omega}{8\pi^3} \right) = \frac{\Omega}{4\pi^3} \quad dk_x dk_y dk_z$$

DOS: k-space vs. energy space



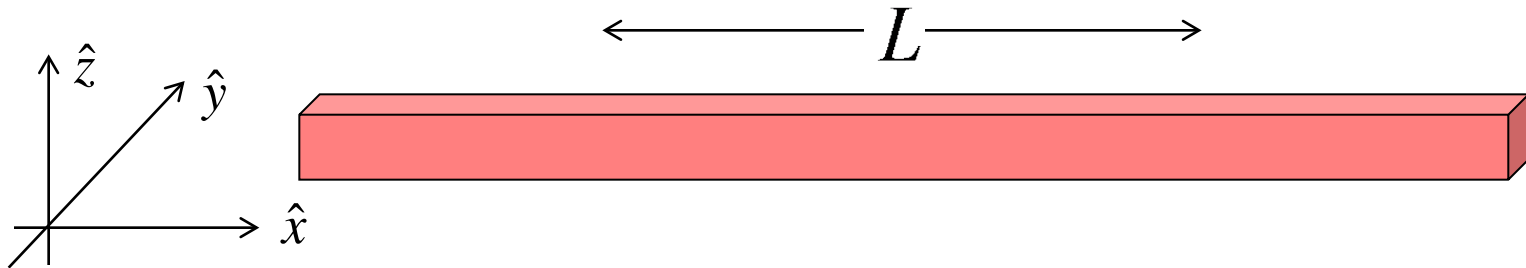
but non-uniformly distributed in energy space.

Depends on $E(k)$
(e.g. different for parabolic bands and linear bands)

$$D'(E)dE = N(k)dk$$

States are uniformly distributed in k-space,

Example 1: DOS(E) for 1D nanowire



Find DOS(E) per unit energy, per unit length, a **single subband** assuming parabolic energy bands.

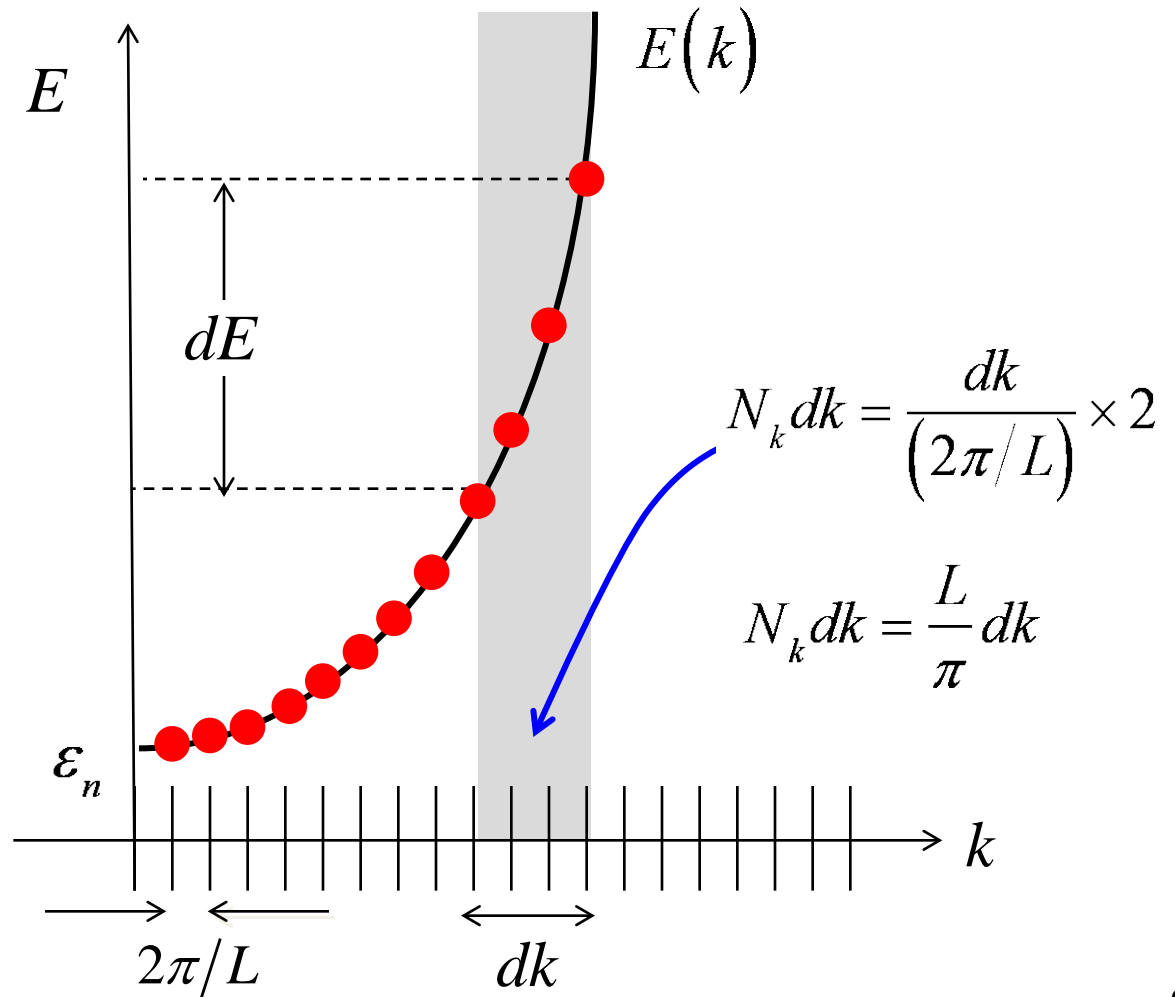
$$E = \varepsilon_n + \frac{\hbar^2 k_x^2}{2m^*}$$

1D (single subband)

$$D'_{1D}(E)dE = N_k dk$$

$$D_{1D}(E)dE = \frac{N_k dk}{L}$$

$$D_{1D}(E) \frac{\#}{\text{J-m}}$$



1D DOS

$$D_{1D}(E)dE = \frac{N_k dk}{L}$$

$$D_{1D}(E)dE = \frac{1}{\pi} dk$$

$$dE = \frac{\hbar^2 k dk}{m^*} \quad k = \frac{\sqrt{2m^*(E - \varepsilon_n)}}{\hbar}$$

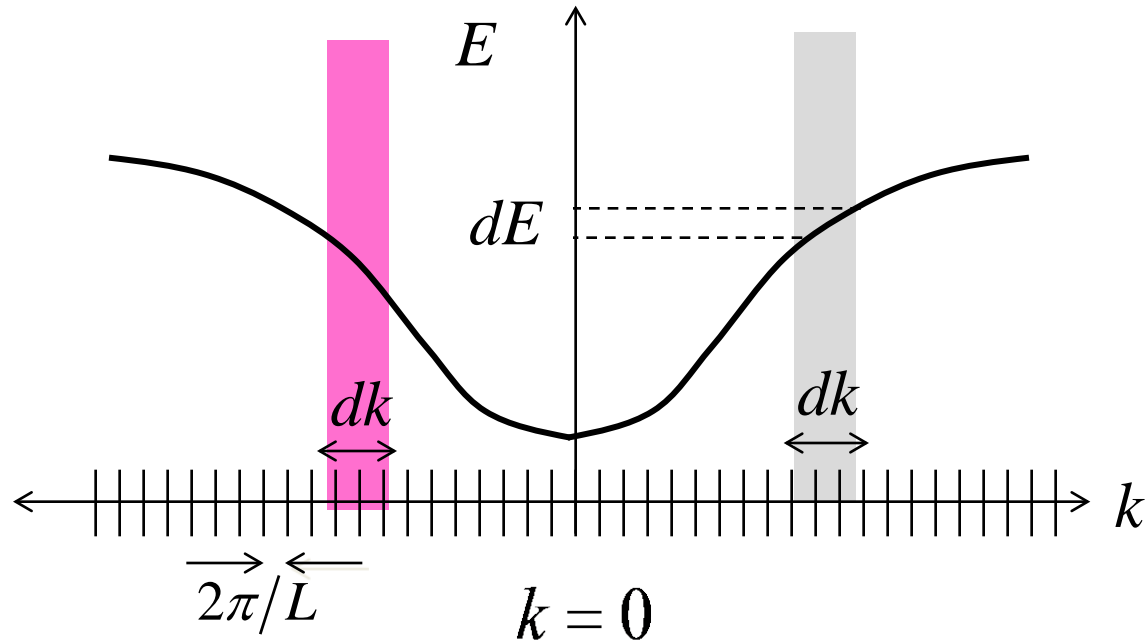
$$D_{1D}(E)dE = \frac{1}{\pi \hbar} \sqrt{\frac{m^*}{2(E - \varepsilon_n)}} dE$$

$E > \varepsilon_n$ DOS in subband, n . $n = 1, 2, 3 \dots$

$$N_k dk = \frac{L}{\pi} dk$$

$$E = \varepsilon_n + \frac{\hbar^2 k^2}{2m^*}$$

Don't forget to multiply by 2

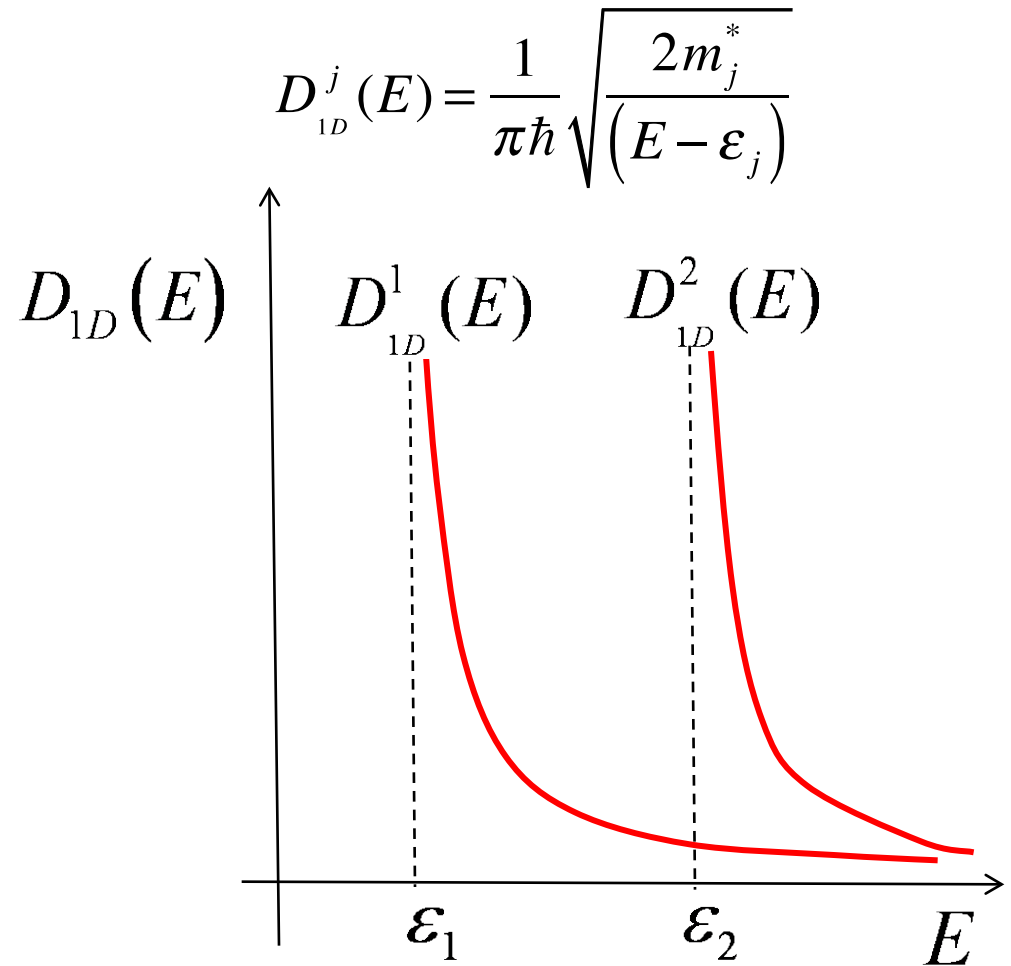
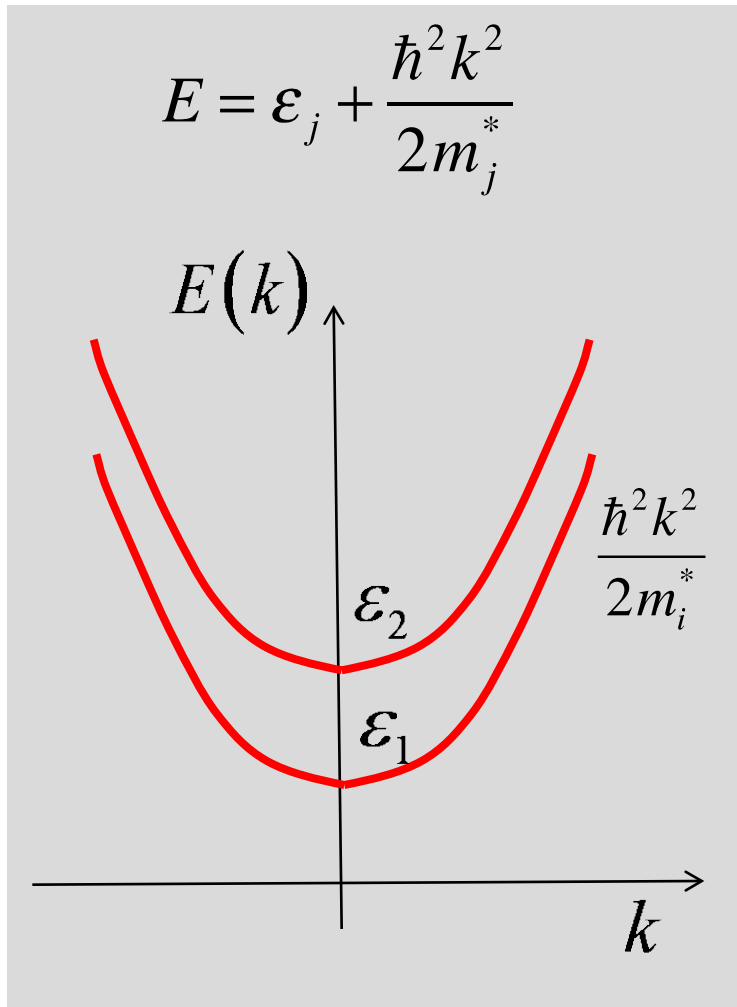


Multiply by 2 to account for the negative k -states.

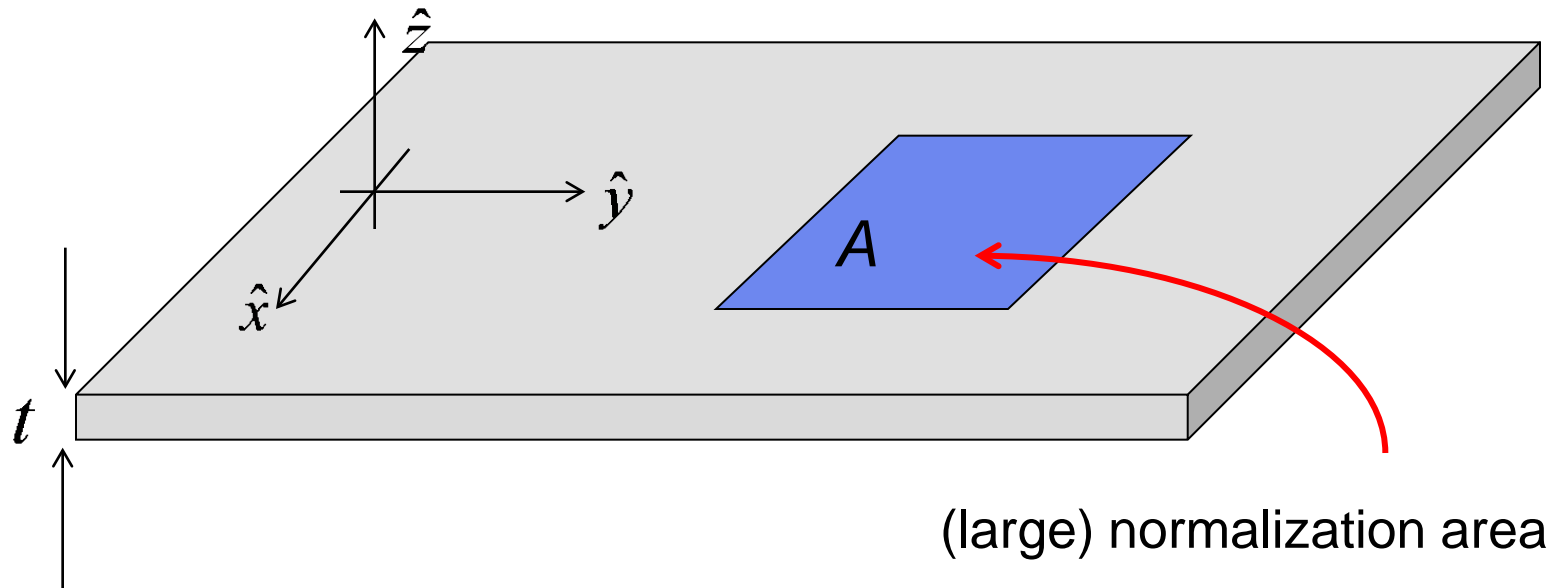
$$D_{1D}(E)dE = \frac{2}{\pi\hbar} \sqrt{\frac{m^*}{2(E - \epsilon_n)}} dE$$

(parabolic energy bands)

Multiple subbands



Example 2: DOS(E) for 2D electrons



Find DOS(E) per unit energy, per unit area, for a **single subband** assuming parabolic energy bands.

$$E = \epsilon_j + \frac{\hbar^2 k_{\parallel}^2}{2m_j^*}$$

Example 2: DOS(E) for 2D electrons

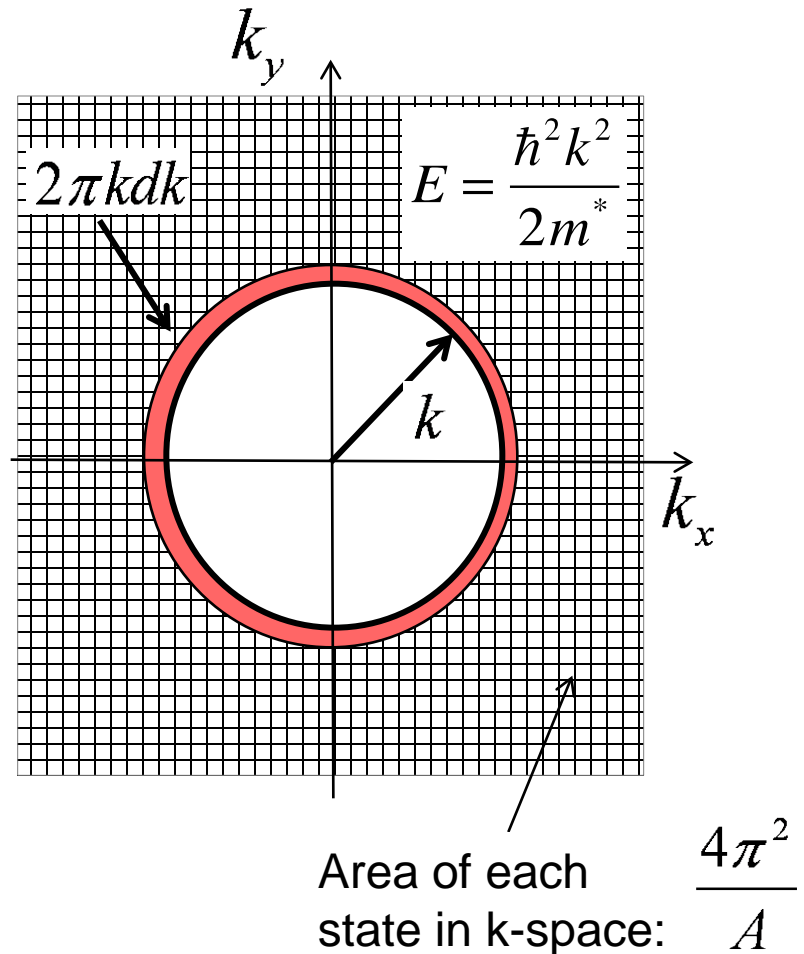
$$D(E)dE = \frac{N(k)}{A} dk^2$$

$$N_k = 2 \times \left(\frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2}$$

$$D(E)dE = \frac{1}{2\pi^2} 2\pi k dk$$

$$E = \epsilon_n + \frac{\hbar^2 k^2}{2m^*} \quad dE = \epsilon_n + \frac{\hbar^2 k dk}{m^*}$$

$$D_{2D}(E) = \frac{m^*}{\pi \hbar^2} \quad E > E_C$$



Example 3: DOS(E) for 3D electrons

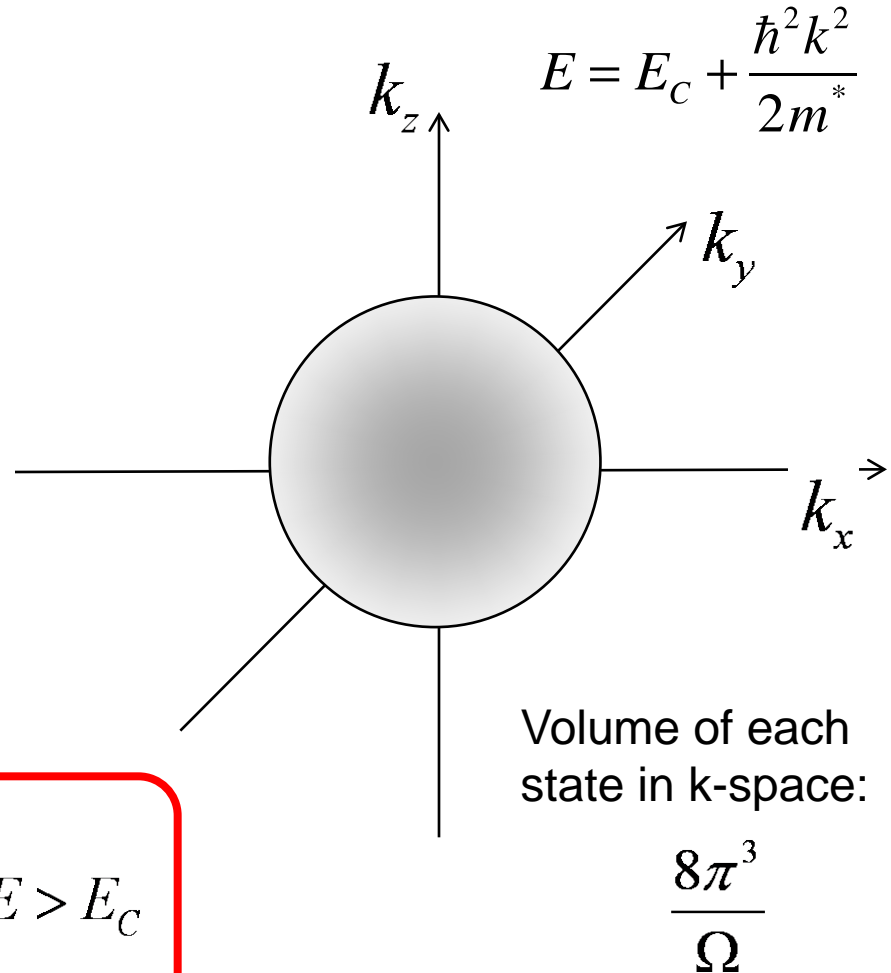
$$D(E)dE = \frac{N(k)}{\Omega} dk^3$$

$$N_k = 2 \times \left(\frac{\Omega}{8\pi^3} \right) = \frac{\Omega}{4\pi^3}$$

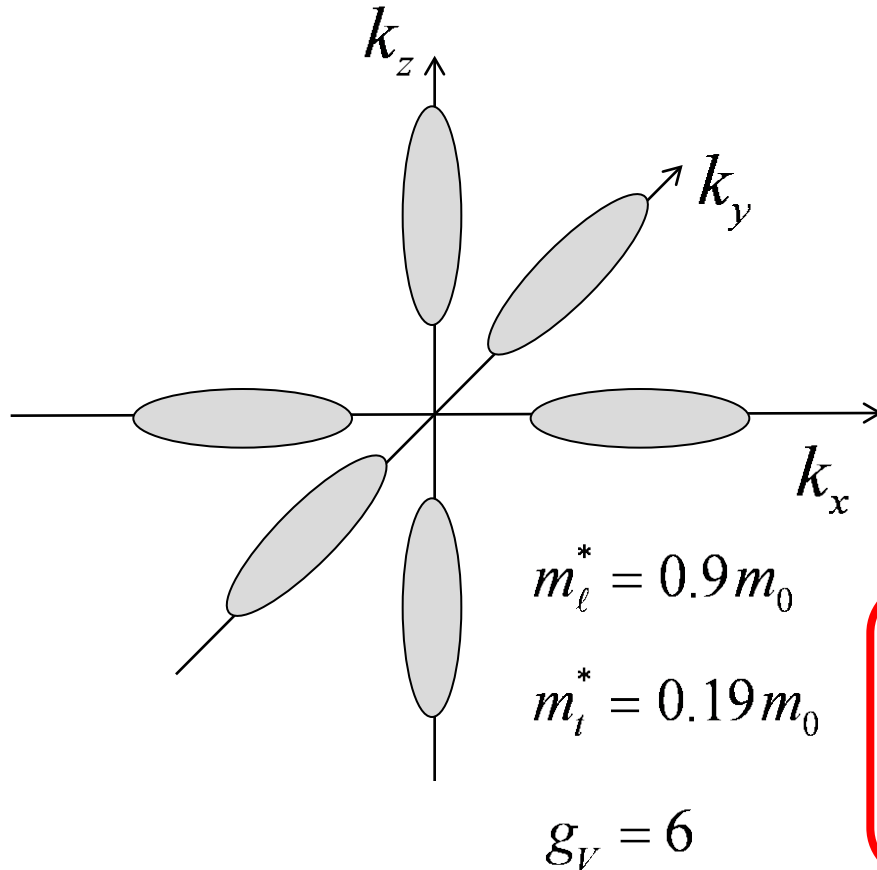
$$D(E)dE = \frac{1}{4\pi^3} 4\pi k^2 dk$$

$$E = E_C + \frac{\hbar^2 k^2}{2m^*}$$

$$D_{3D}(E) = \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2 \hbar^3} \quad E > E_C$$



Ellipsoidal band and valley degeneracy



$$D_{3D}(E) = \frac{m^* \sqrt{2m^*(E - E_C)}}{\pi^2 \hbar^3} \quad m^* = ?$$

$$m_D^* \equiv 6^{2/3} (m_l m_t^2)^{1/3}$$

$$D_{3D}(E) = \frac{m_D^* \sqrt{2m_D^*(E - E_C)}}{\pi^2 \hbar^3}$$

Conduction band of Si:
6 equivalent ellipsoidal valleys:

Comments on 3D DOS

$$D_{3D}(E) = \frac{m_D^* \sqrt{2m_D^* (E - E_C)}}{\pi^2 \hbar^3}$$

For a bulk semiconductor with parabolic bands:

$$D_{3D}(E) \propto (m_D^*)^{3/2}$$

$$D_{3D}(E) \propto \sqrt{(E - E_C)}$$

Si: $m_D^* = 1.182m_0$

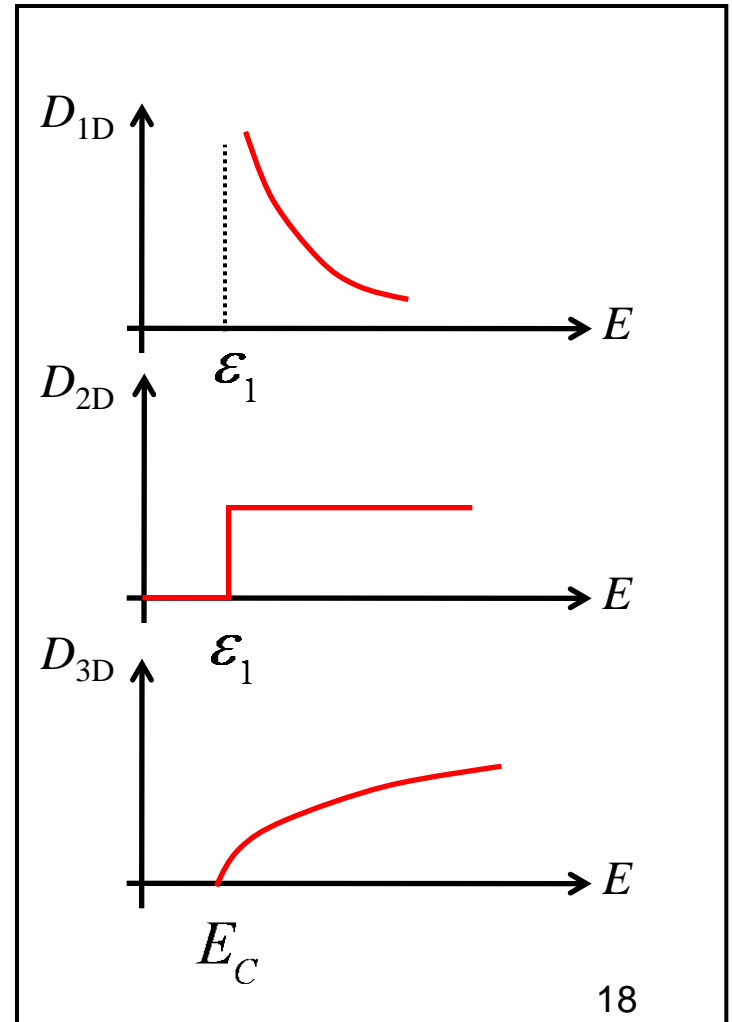
GaAs: $m_D^* = 0.0655m_0$

Parabolic bands: 1D, 2D, and 3D

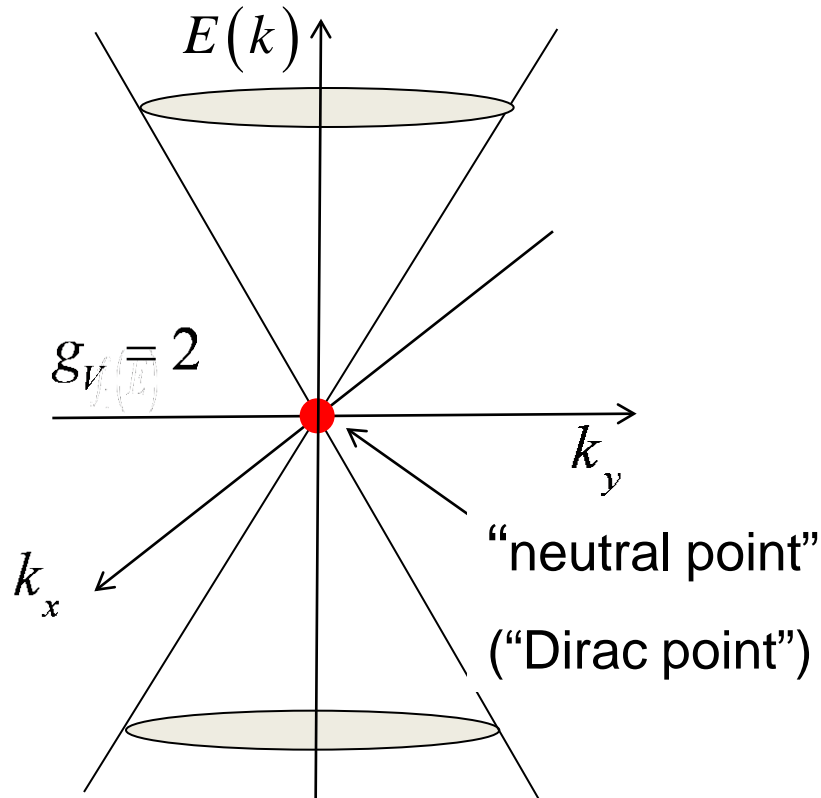
$$D_{1D}(E) = g_V \frac{1}{\pi \hbar} \sqrt{\frac{2m^*}{(E - \varepsilon_1)}} \Theta(E - \varepsilon_1)$$

$$D_{2D}(E) = g_V \frac{m^*}{\pi \hbar^2} \Theta(E - \varepsilon_1)$$

$$D_{3D}(E) = g_V \frac{m^* \sqrt{2m^* (E - E_C)}}{\pi^2 \hbar^3} \Theta(E - E_C)$$

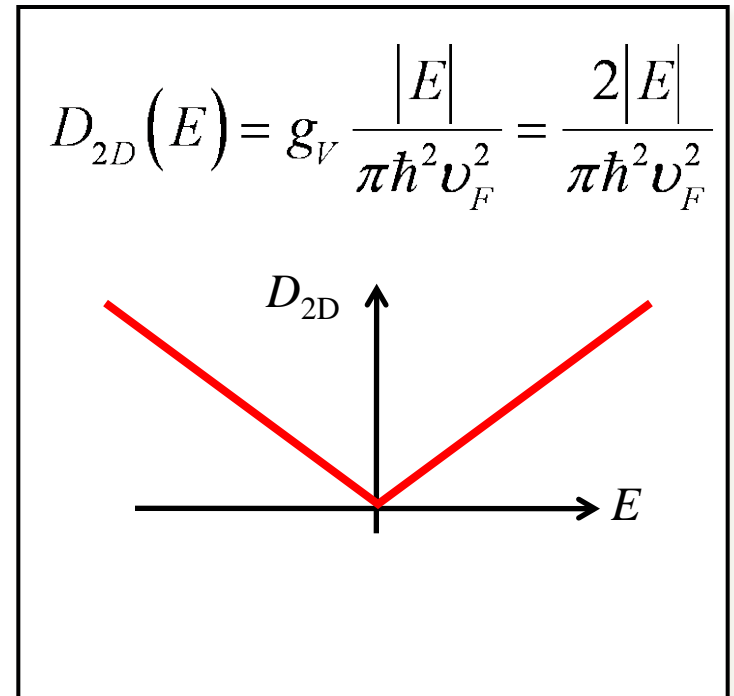


Exercise



$$E(k) = \pm \hbar v_F k = \pm \hbar v_F \sqrt{k_x^2 + k_y^2}$$

Show that for graphene, the 2D DOS is:



Summary

The DOS is an important concept – one that we will use frequently in the next unit.

The DOS depends on dimension.

$DOS(k)$ is constant, but $DOS(E)$ depends on the band structure.

For 3D, bulk semiconductors with parabolic bands,
 $DOS \sim (m^*)^{3/2}$ and $DOS \sim \text{sqrt}(E - E_C)$