Density of States

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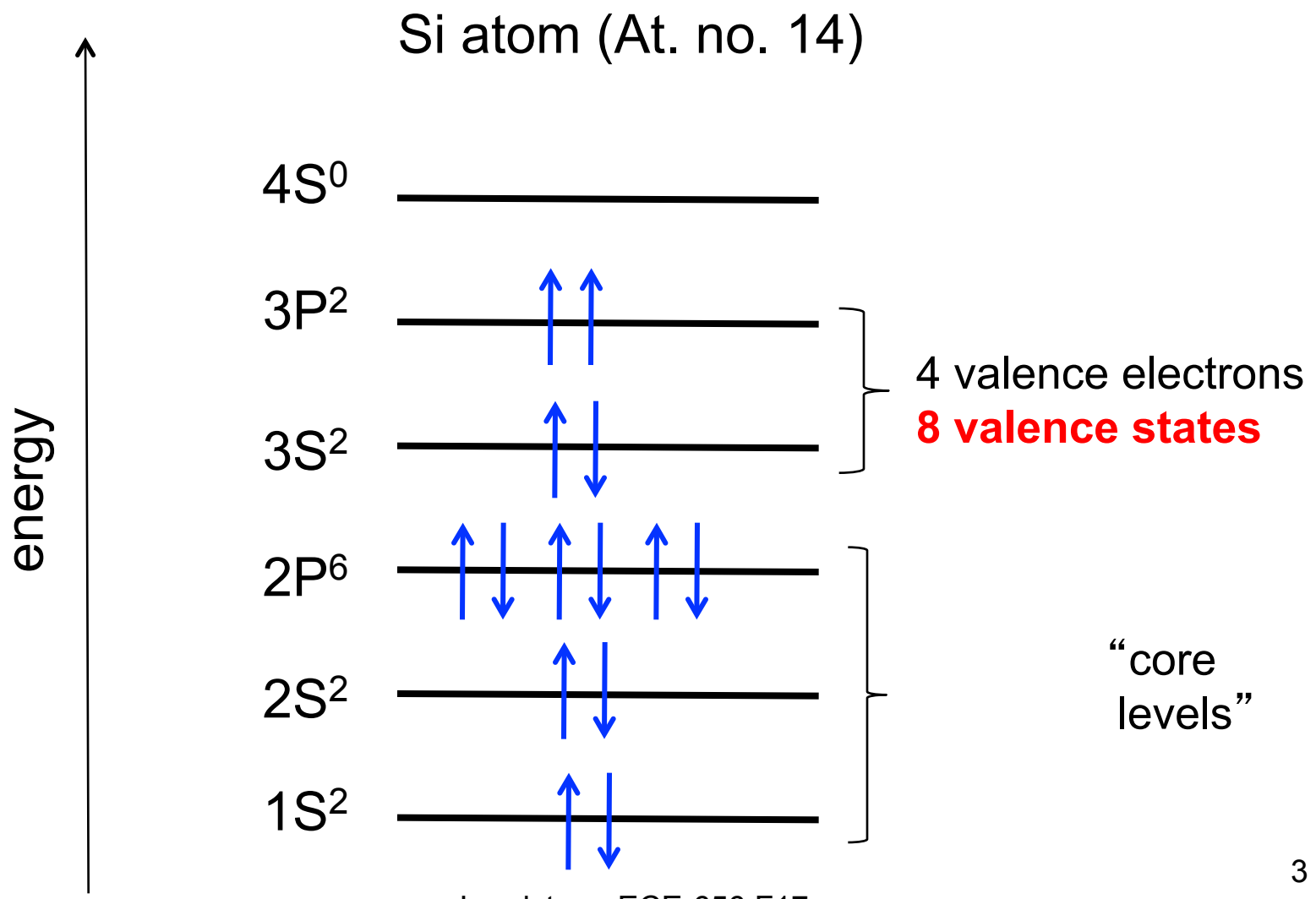
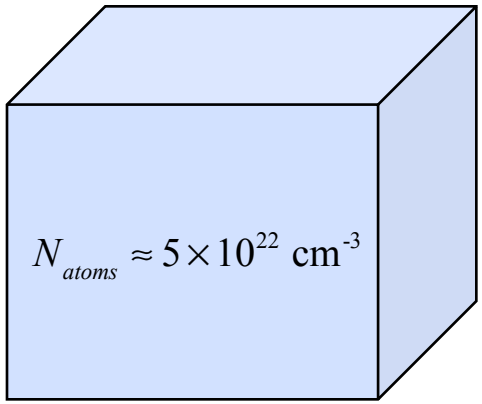
Outline

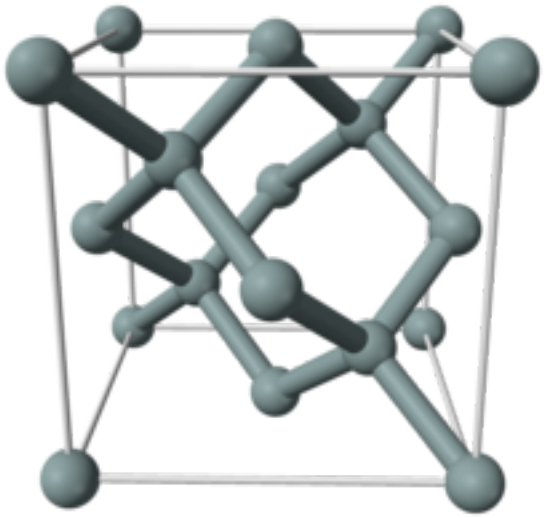
1) Counting states
2) DOS in k-space vs. DOS in E-space
3) Examples
4) Realistic DOS in semiconductors
5) DOS for phonons

Energy levels in Si



States in a Si crystal

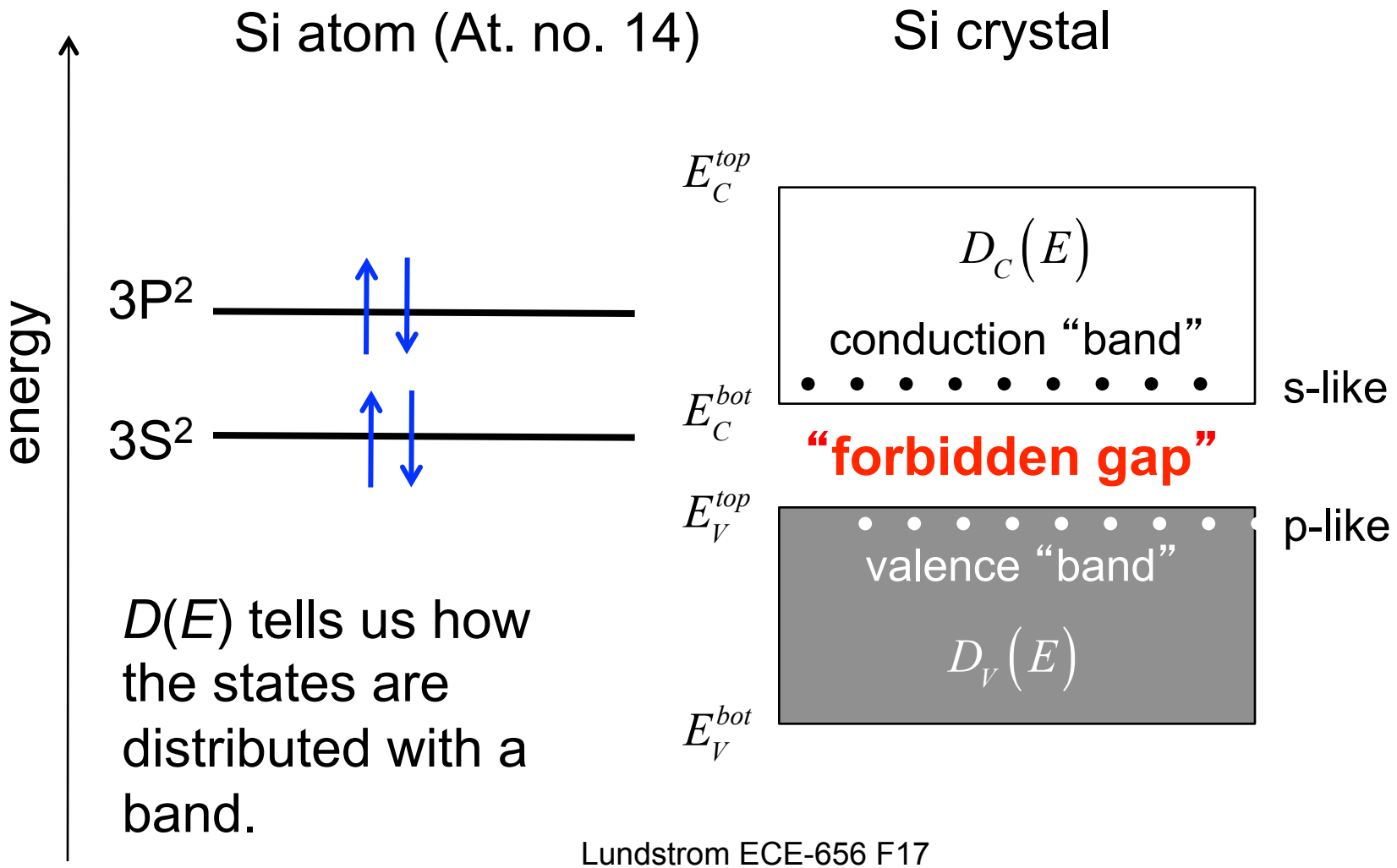




5.43 A

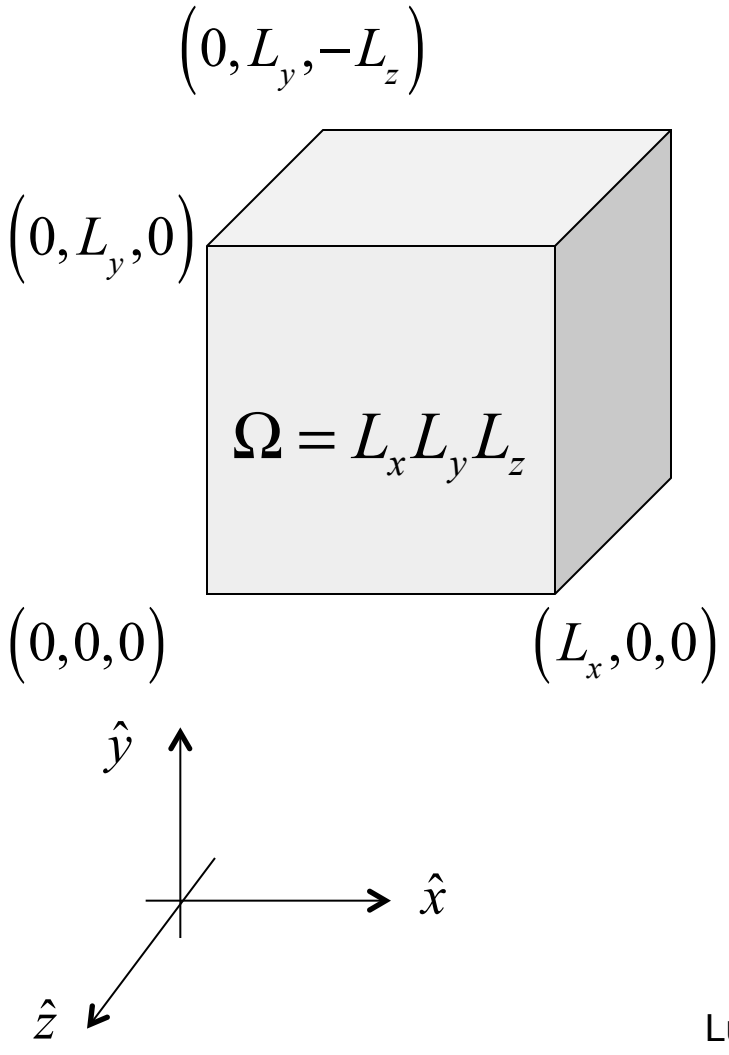
- Only the valence states are of interest to us.
- 3s and 3p orbitals hybridize and produce bonding and anti-bonding states.
- The interaction of the electron wavefunctions in the crystal broadens the discrete energy levels of the isolated Si atoms into energy bands.

Energy levels → energy bands



D(*E*) tells us how the states are distributed with a band.

States in a finite volume of semiconductor



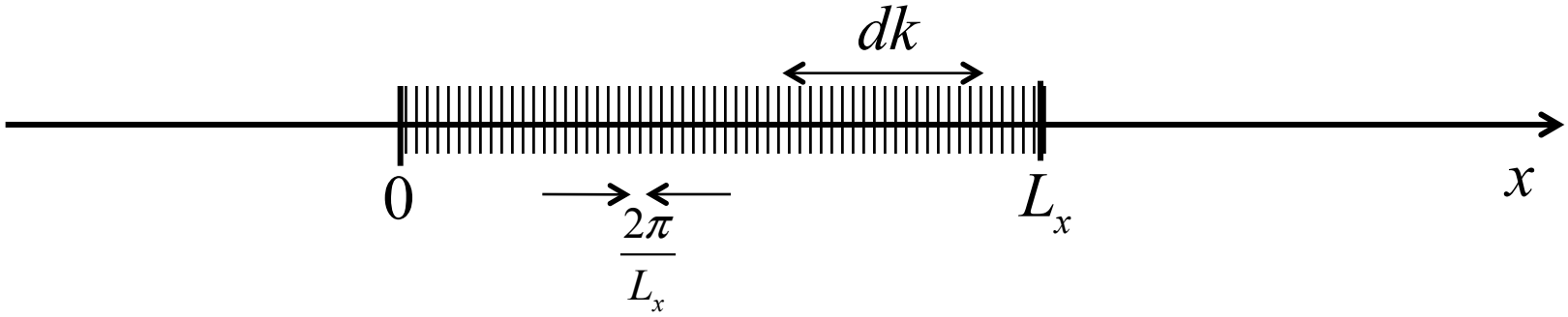
Finite volume, Ω
(***part of an infinite volume***)

Finite number of states

Periodic boundary conditions:

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

x-direction



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

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

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

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

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

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

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

"Brillouin zone" $\quad 0 < k < \frac{2\pi}{a} \qquad k_{\max} = \frac{2\pi}{a}$

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Density-of-states in k-space

1D:

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

2D:

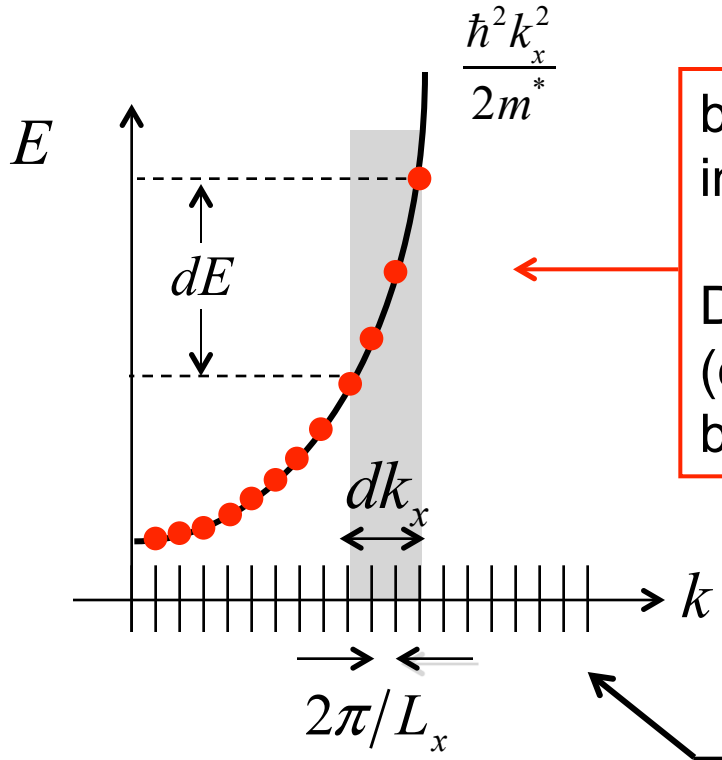
$$N_k = 2 \times \left(\frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} \qquad dk_x dk_y$$

independent of *E*(*k*)

3D:

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

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)

States are uniformly distributed in k-space,

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

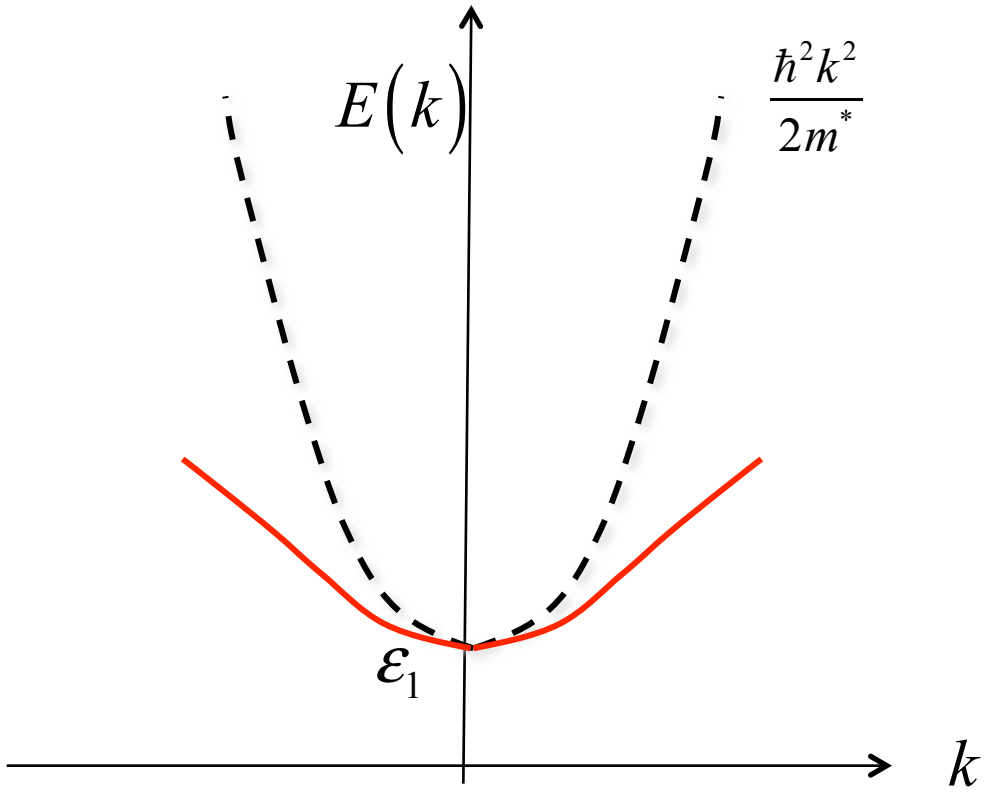
Effect of E(k) on the DOS

How does non-parabolicity affect DOS(E)?

"Kane bands"

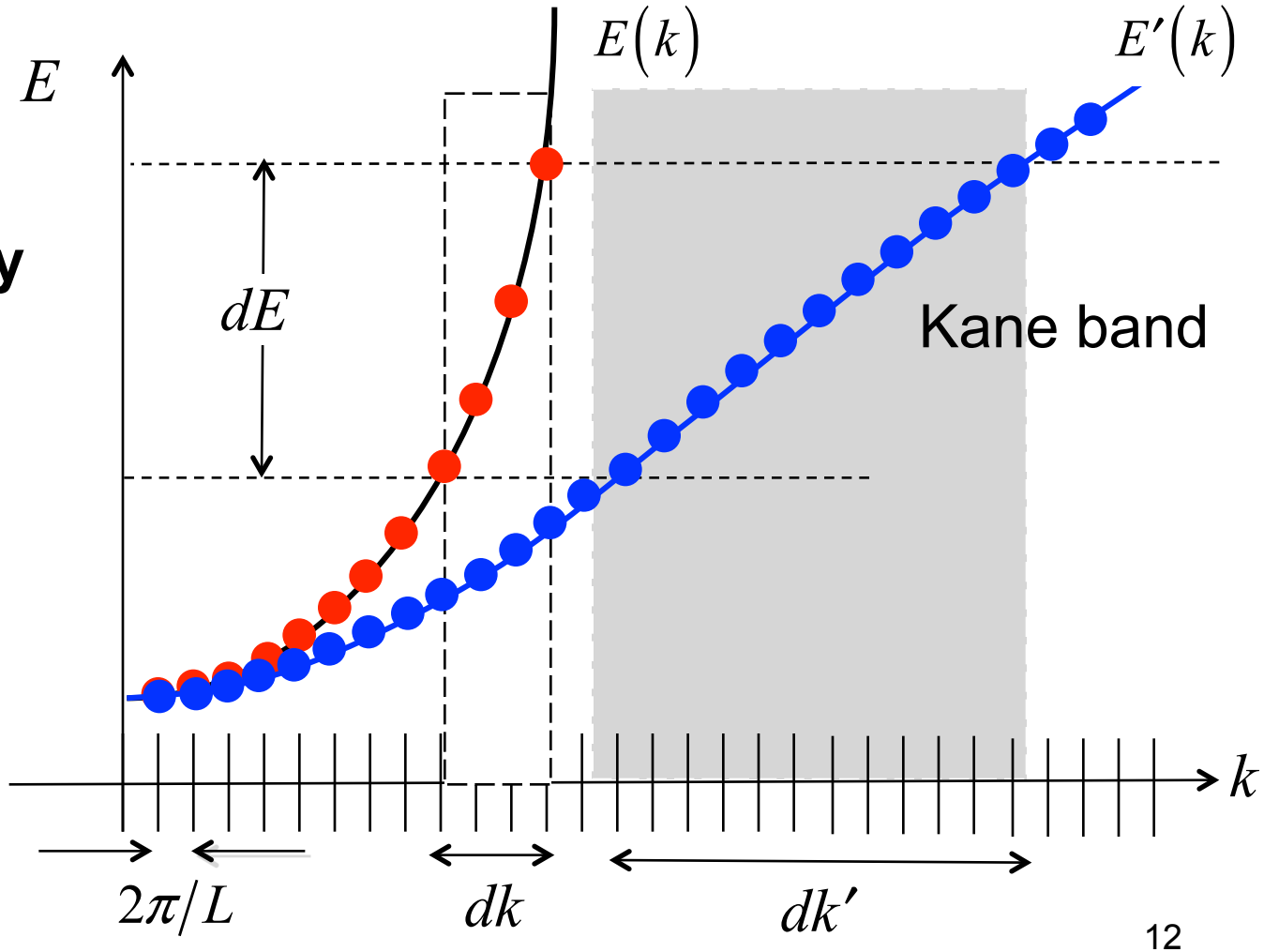
$$E'\left(1+\alpha E'\right)=\frac{\hbar^2 k^2}{2m^*(0)}$$

$$E' = E - \varepsilon_1$$



Effect on DOS

Nonparaboliciy increases the DOS (E).



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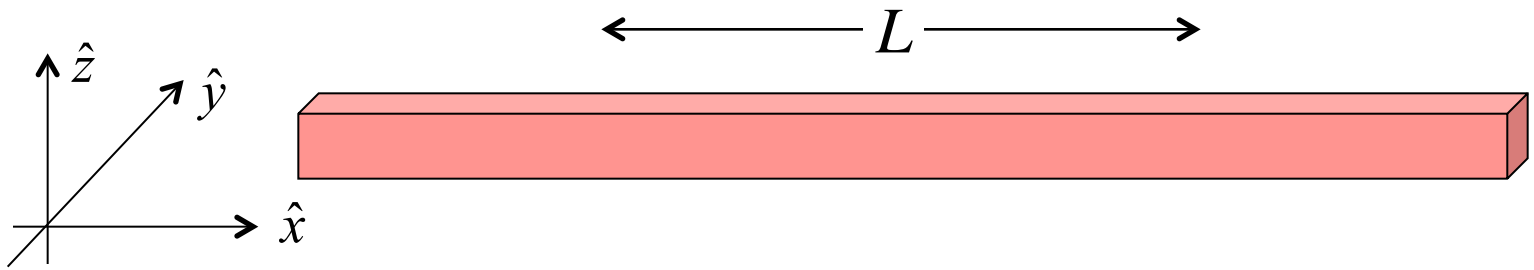
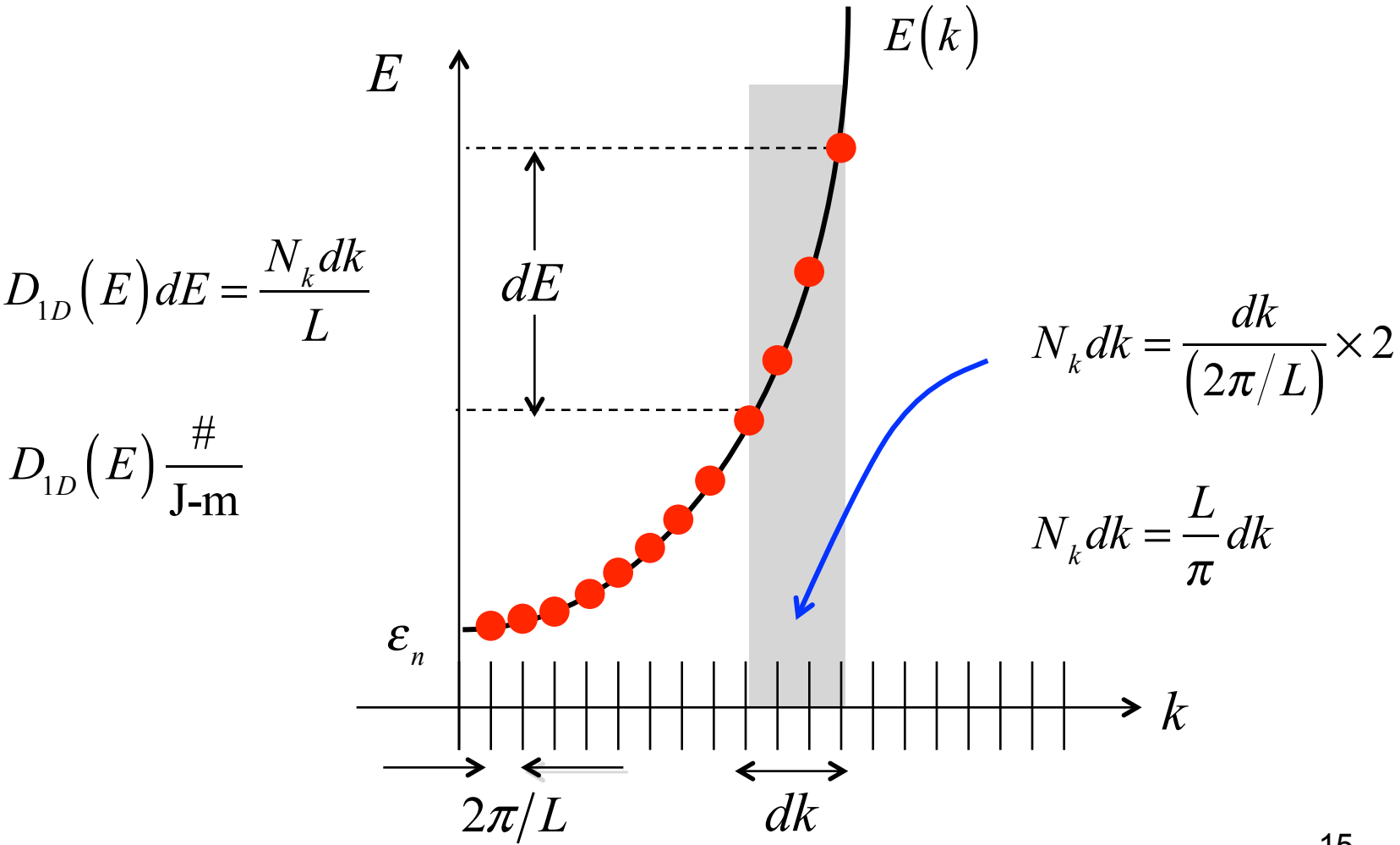
DOS(E) for 1D nanowire



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

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

Example: 1D (single subband)



1D DOS

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

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

$$dE = \frac{\hbar^2 k dk}{m^*} \qquad dk = \frac{m^* dE}{\hbar^2 k}$$

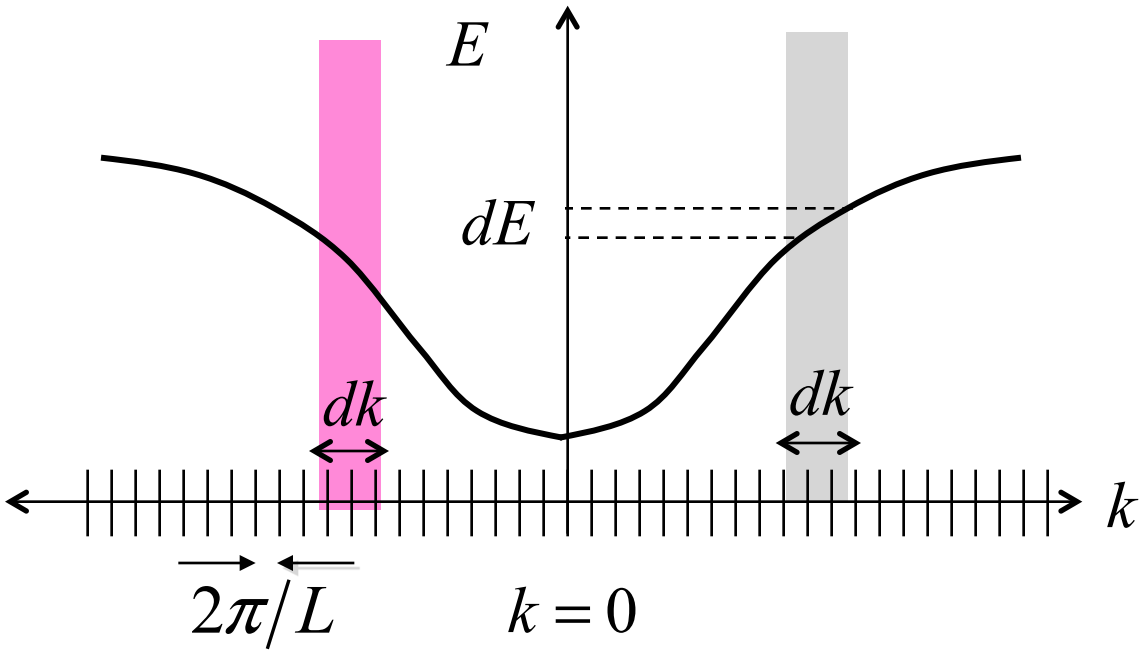
$$k = \frac{\sqrt{2m^*\left(E-\varepsilon_n\right)}}{\hbar}$$

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

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

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

Don’t forget to multiply by 2



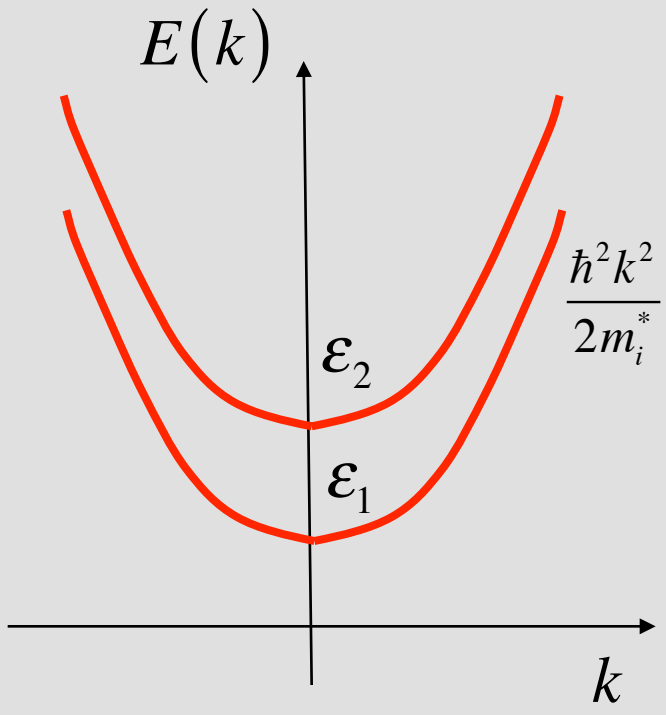
Multiply by 2 to account for the negative k-states.

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

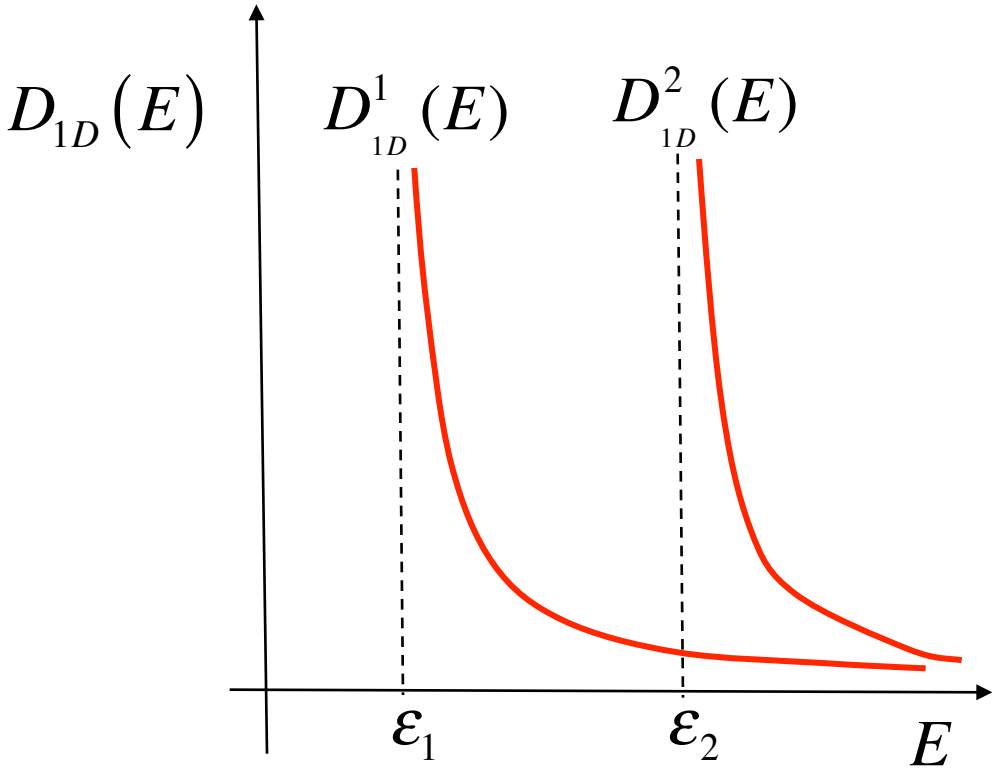
(parabolic energy bands)

Multiple subbands

$$E = \varepsilon_i + \frac{\hbar^2 k^2}{2m_i^*}$$



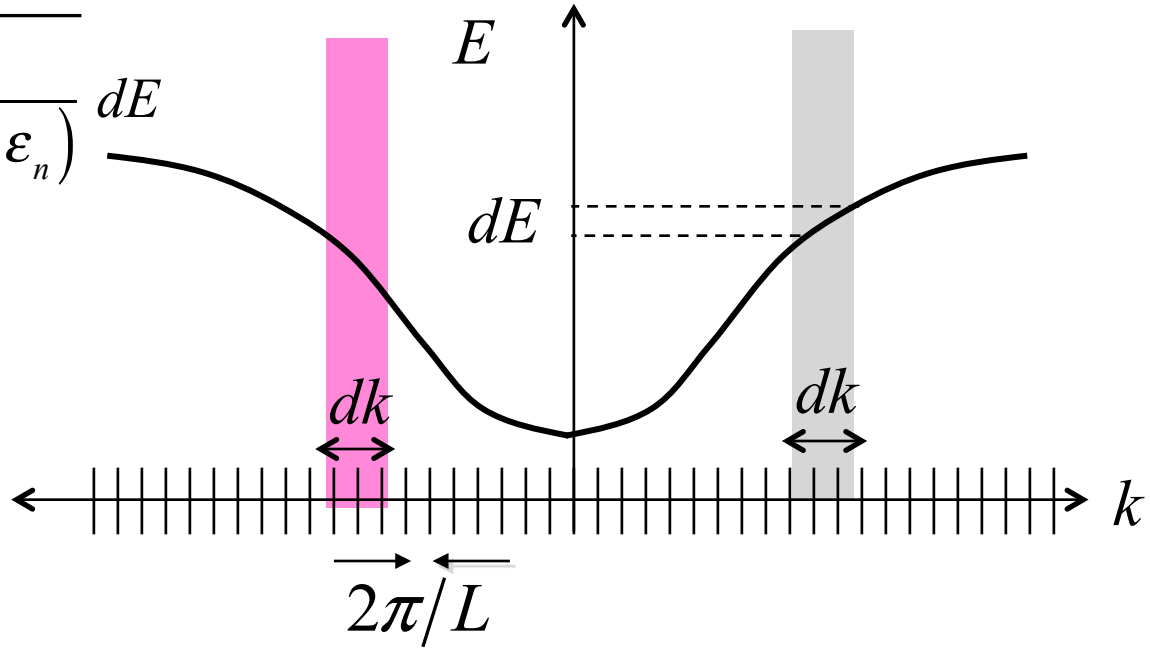
$$D_{1D}^{n}(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m_i^*}{(E-\varepsilon_n)}}$$



In terms of velocity

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

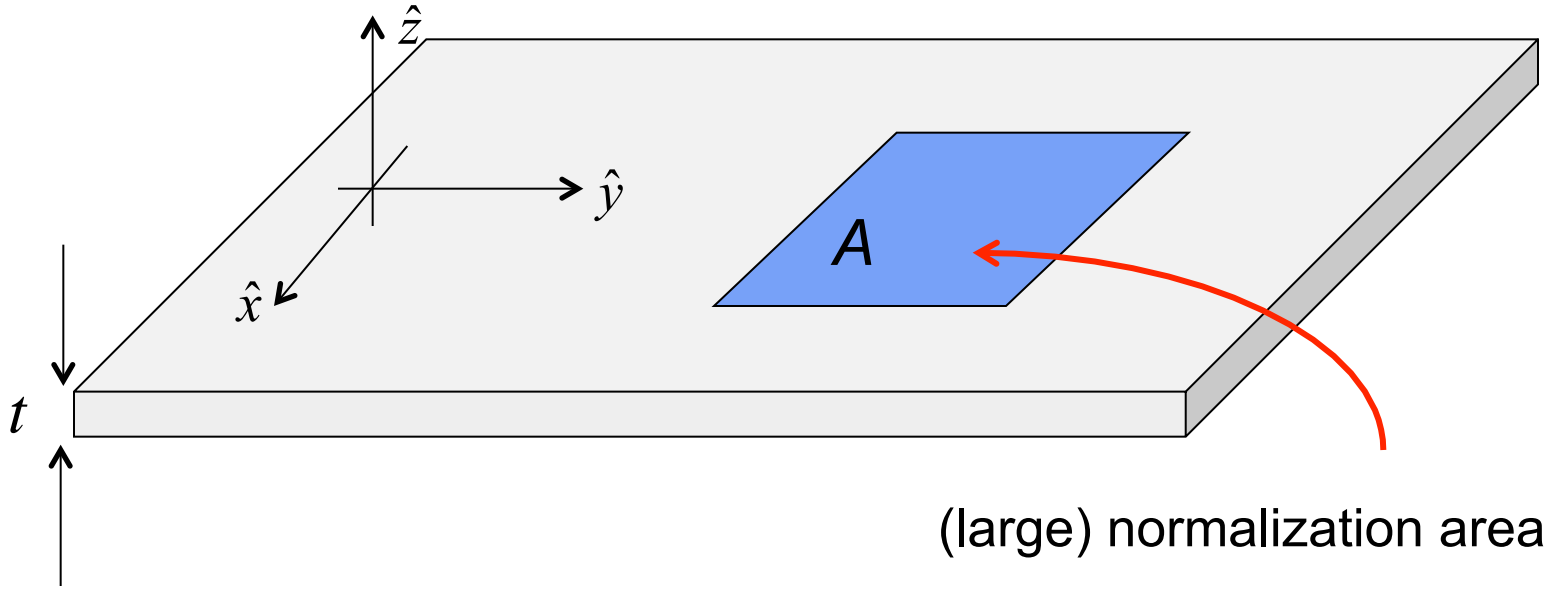
$$\upsilon = \frac{\hbar k}{m^*} = \sqrt{2(E-\varepsilon_n)/m^*}$$



$$D_{1D}(E)dE = \frac{2}{\pi\hbar\upsilon}dE$$

Exercise: Show that the final expression is independent of bandstructure.

Example 2: DOS(E) for 2D electrons



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

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

Example 2: DOS(E) for 2D electrons

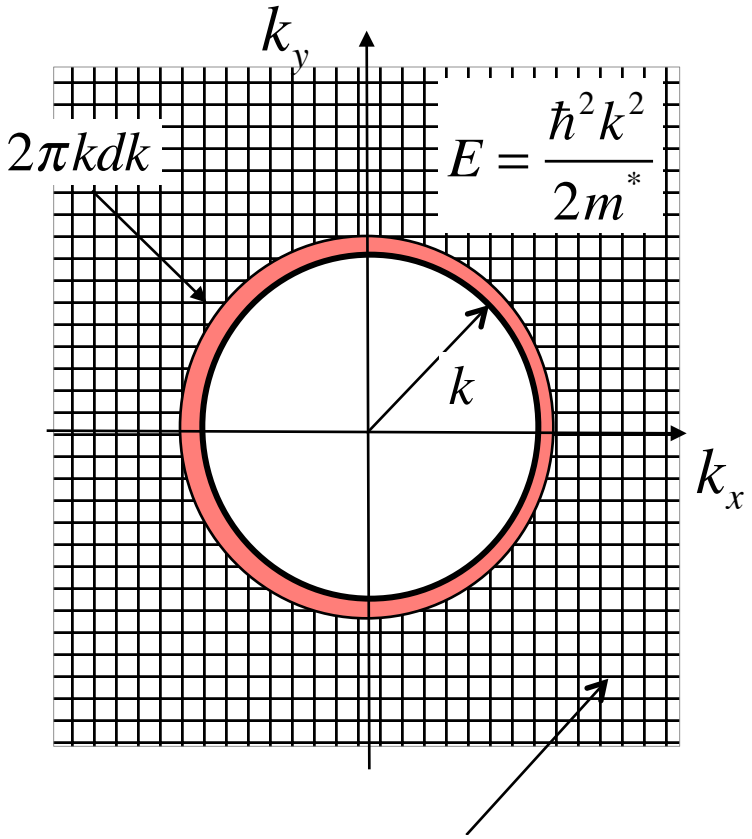
$$D(E)dE = \frac{N(k)}{A}dk^2$$

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

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

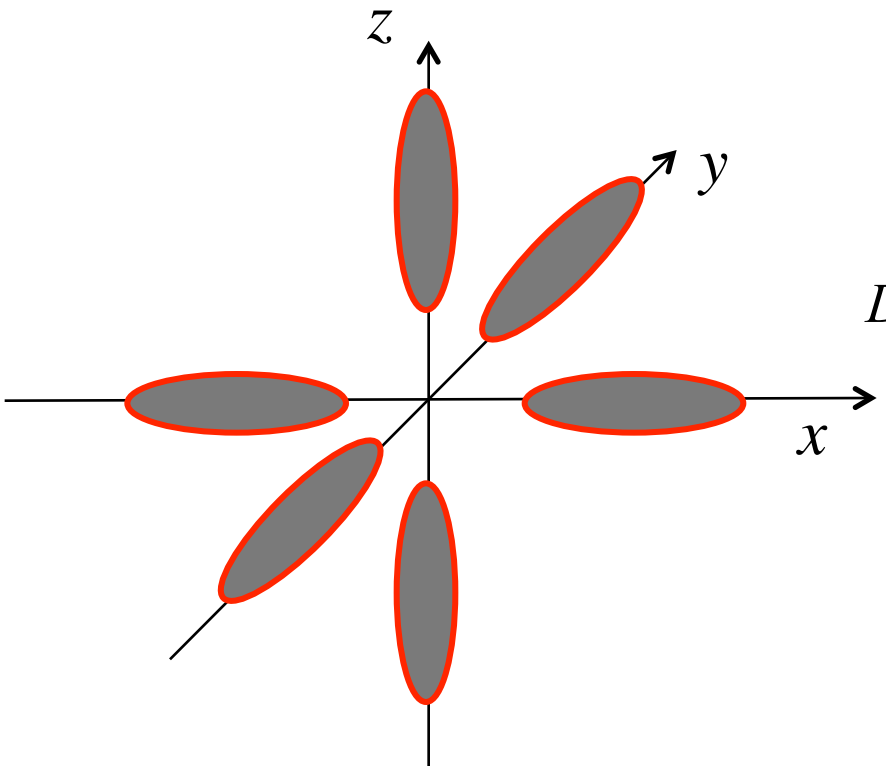
Exercise: Show that:

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



Area of each state in k-space: $\frac{4\pi^2}{A}$

Valley degeneracy



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

$$\Rightarrow g_V \frac{m_D^* \sqrt{2m_D^*(E - E_C)}}{\pi^2 \hbar^3} \Theta(E - E_C)$$

$$m_D^* \equiv \left(m_\ell m_t^2\right)^{1/3}$$

Conduction band of Si:
6 equivalent valleys: $g_V = 6$ (bulk)

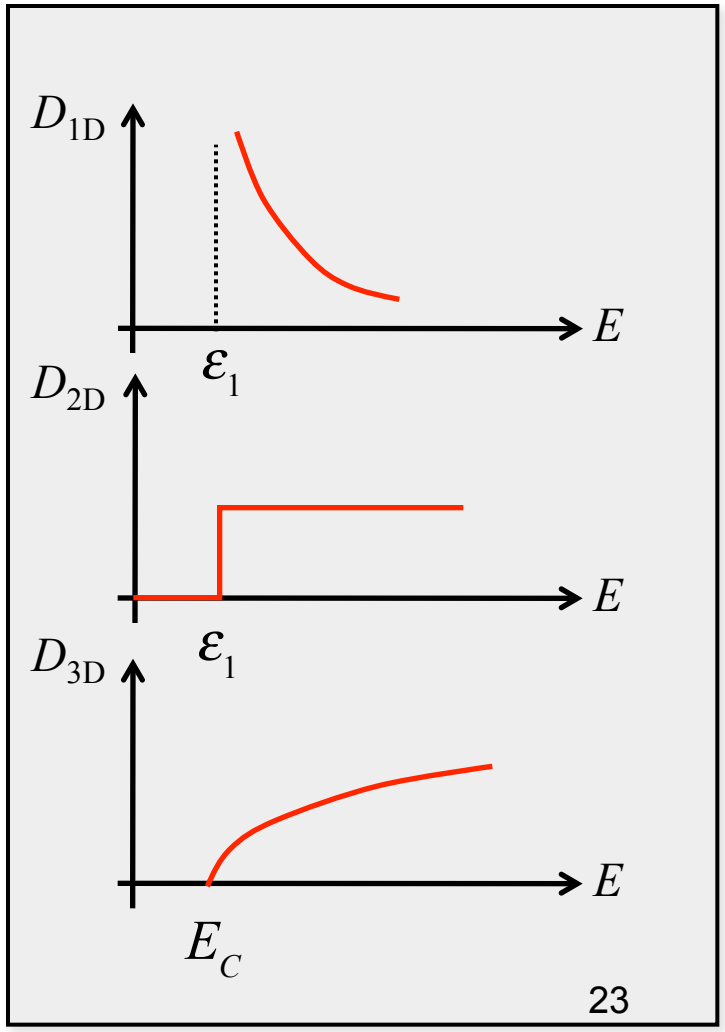
Parabolic bands: 1D, 2D, and 3D

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

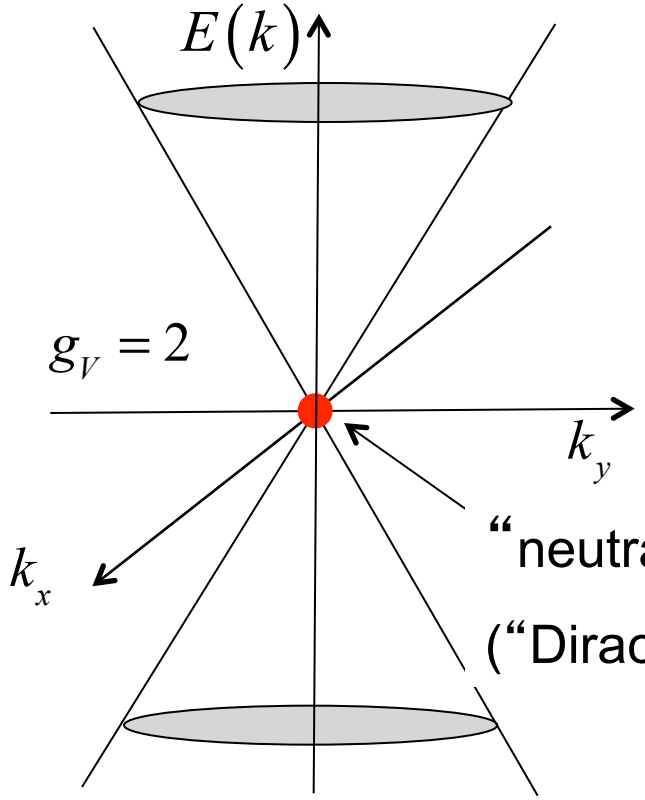
$$D_{2D}(E) = g_V \frac{m^*}{\pi\hbar^2}\Theta(E-\varepsilon_1)$$

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

$$\left(E(k) = E_C + \hbar^2k^2/2m^*\right)$$



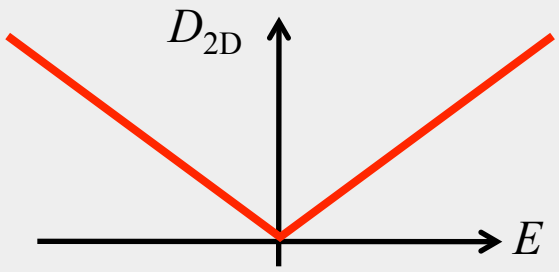
Graphene (2D)



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

Exercise: Show that for graphene, the 2D DOS is:

$$D_{2D}(E) = g_V\frac{|E|}{\pi\hbar^2\upsilon_F^2} = \frac{2|E|}{\pi\hbar^2\upsilon_F^2}$$



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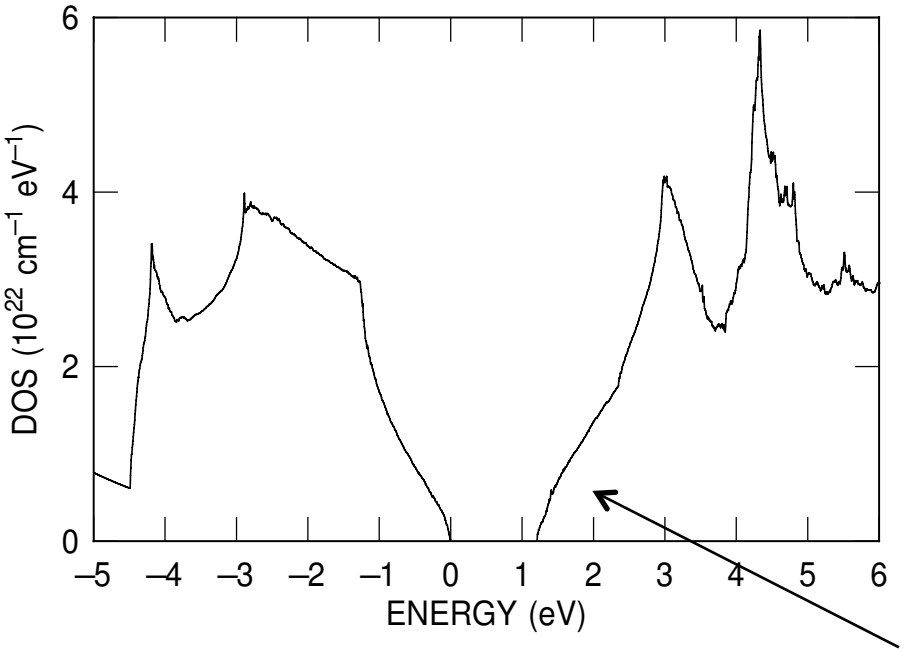
DOS for bulk Si



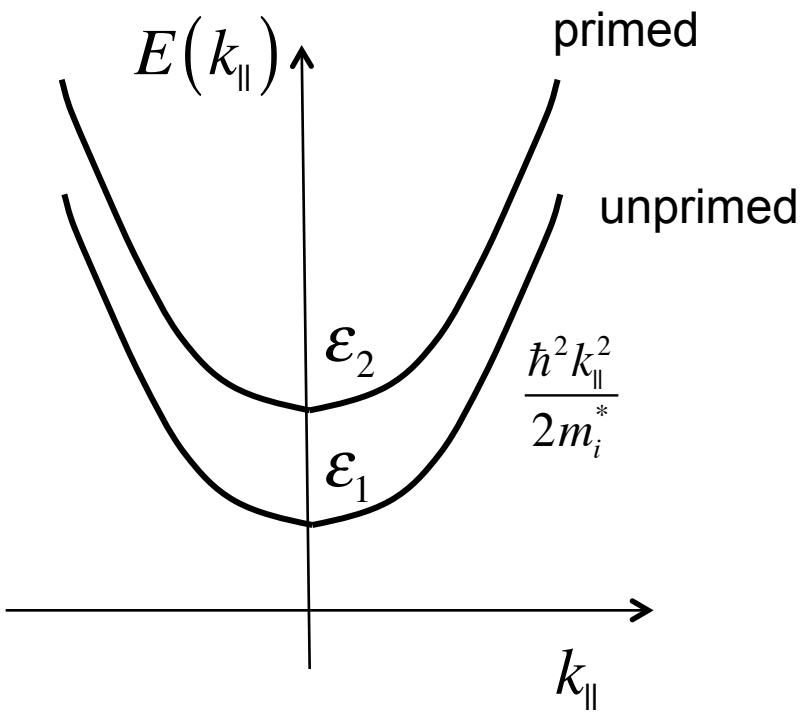
$$D(E) \propto \sqrt{E - E_C}$$

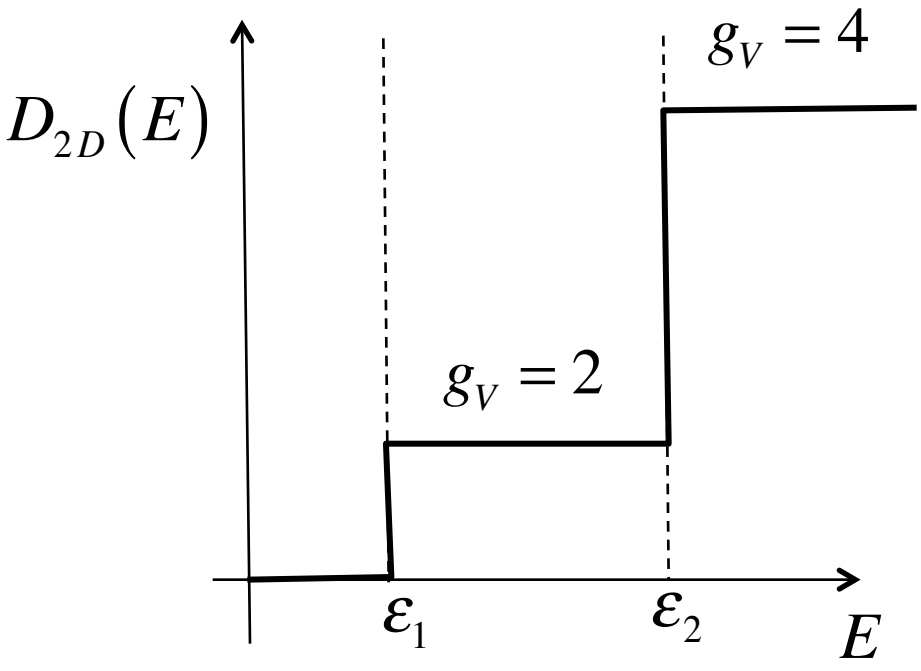
The DOS is calculated with nonlocal empirical pseudopotentials including the spin-orbit interaction. (Courtesy Massimo Fischetti, August, 2011.)

DOS for a Si quantum well

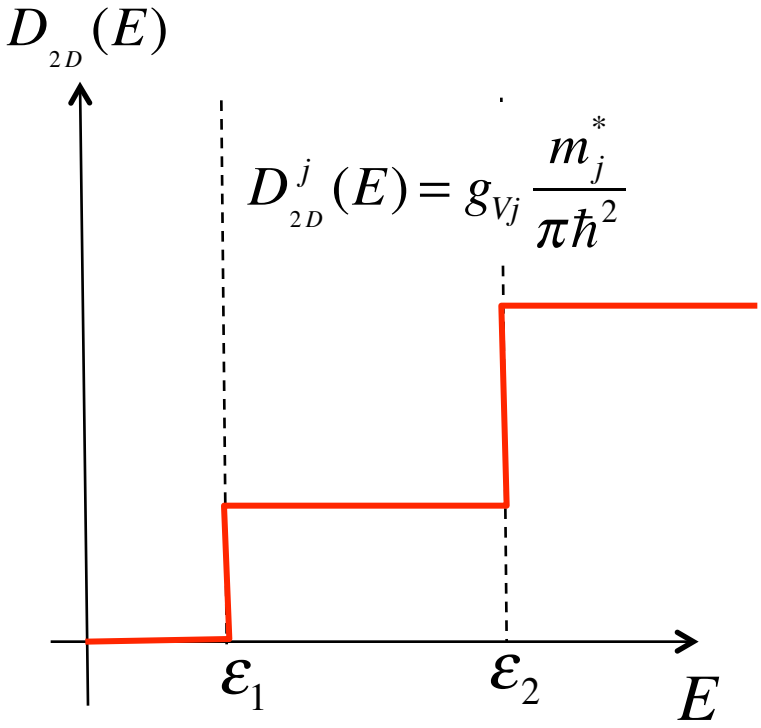
$$E = \varepsilon_j + \frac{\hbar^2 k_{||}^2}{2m_n^*}$$

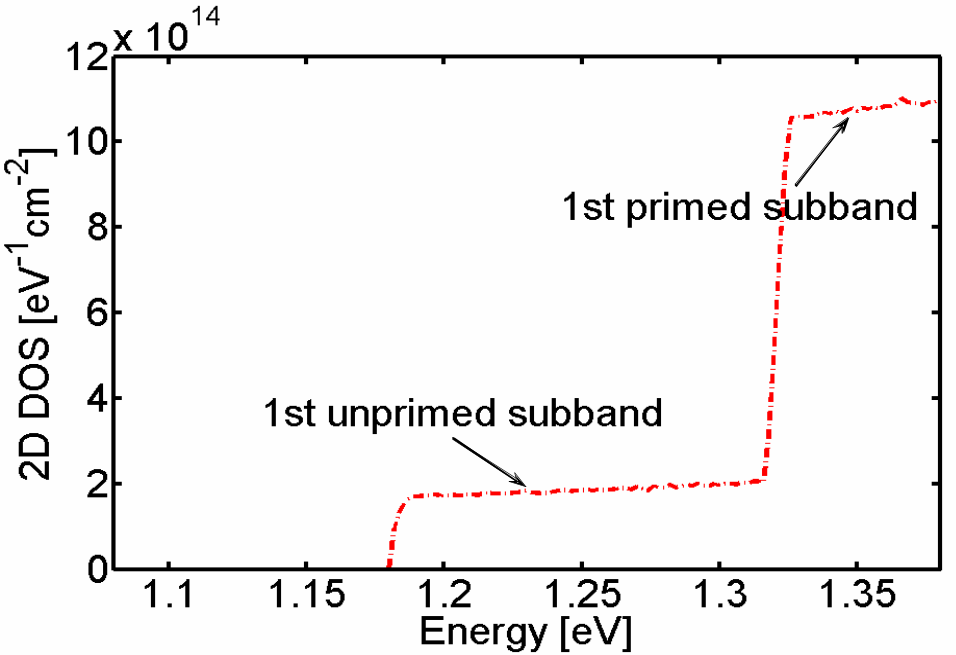
$$D_{2D}^j(E) = g_{Vj}\frac{m_n^*}{\pi\hbar^2}$$





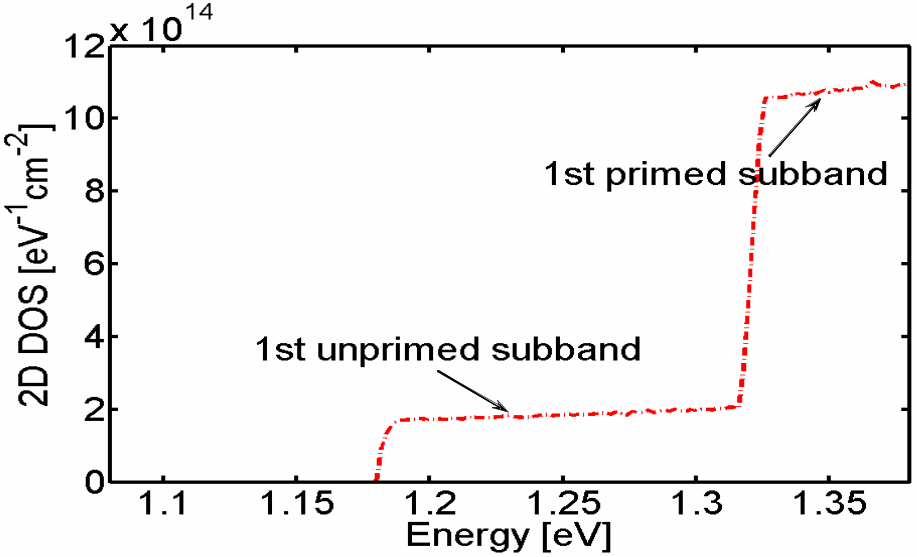
DOS for a Si quantum well

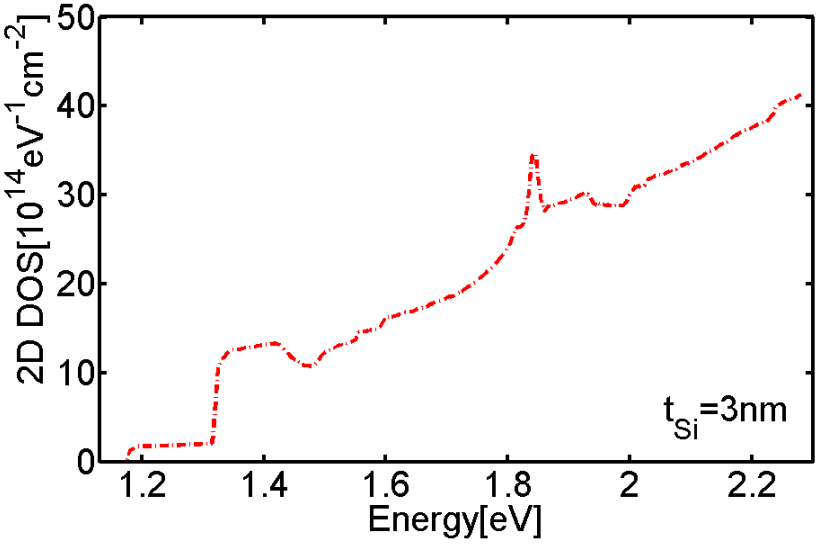




$sp^3s^*d^5$ TB calculation by Yang Liu, Purdue University, 2007

DOS for a Si quantum well





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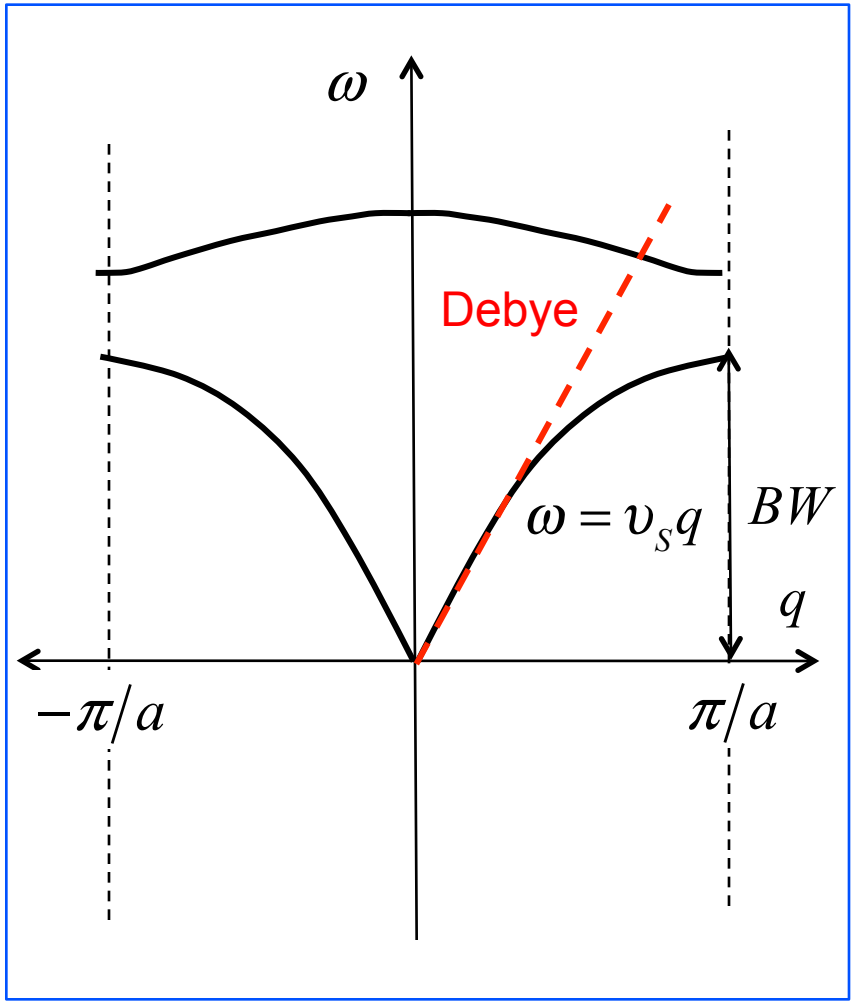
Debye model

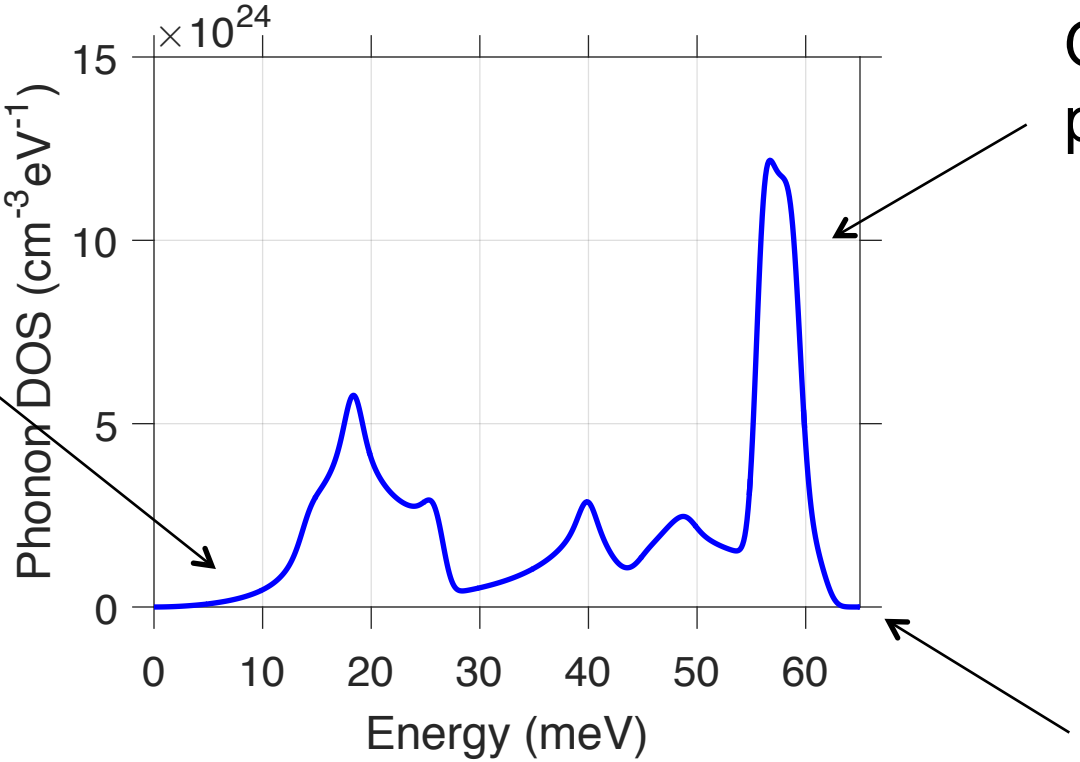


Exercise: Show that the DOS for 3D phonons assuming a linear dispersion is

$$D_{ph}(\hbar\omega) = \frac{3(\hbar\omega)^2}{2\pi^2(\hbar\upsilon_S)^3} \quad \left(\text{J-m}^3\right)^{-1}$$

Realistic phonon DOS (Si)

$D_{ph}(\hbar\omega) \propto E^2$



Optical phonons

Near room temperature and above, **all** states are occupied.

BW only a few kT!

(Figure provided by J. Maassen, Dalhousie Univ., CA, 2017)

Summary

1) DOS in energy depends on dimension **and** on the dispersion.

2) The DOS becomes complicated at high energies.

3) The phonon DOS is generally complicated over the relevant energy range.