ECE 656: Electrothermal Transport in Semiconductors Fall 2015

Density of States

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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:

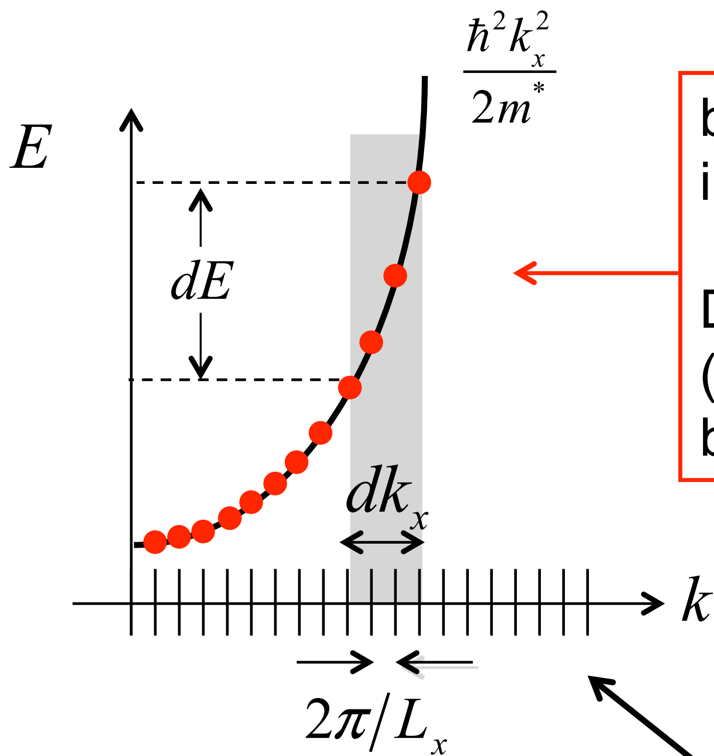
$$N_k = 2 \times \left(\frac{A}{4\pi^2} \right) = \frac{A}{2\pi^2} \qquad dk_x dk_y$$

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



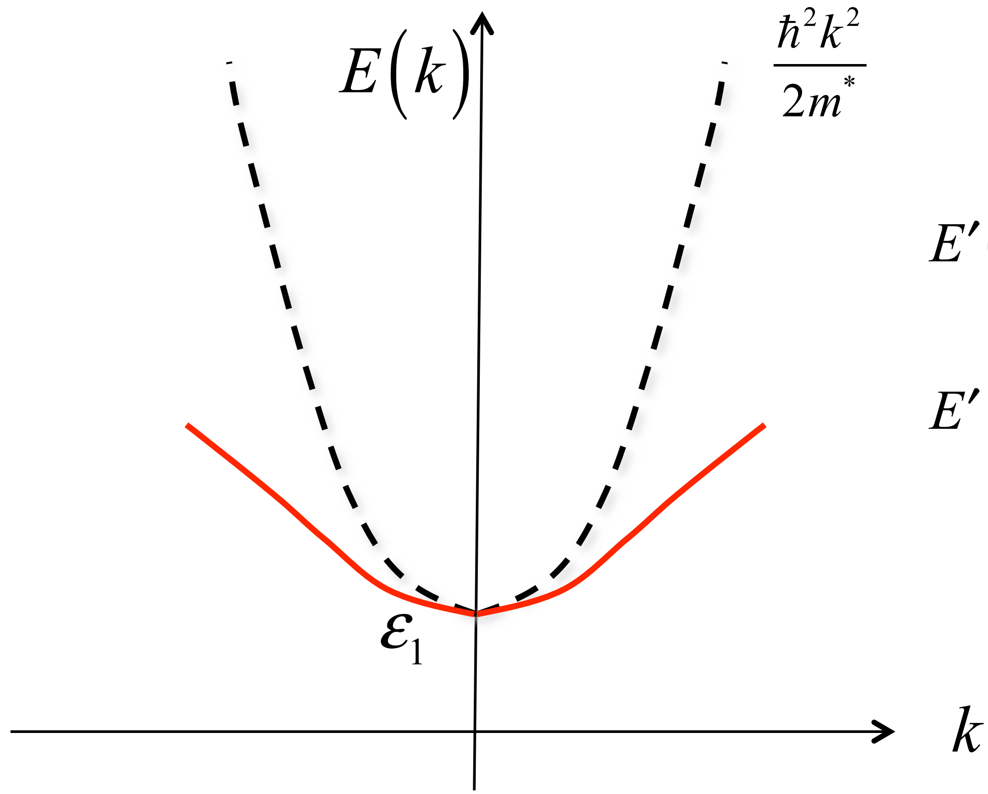
but non-uniformly distributed in energy space.

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

States are uniformly distributed in k-space,

$$\boxed{D(E)dE = N(k)dk}$$

conduction band non-parabolicity

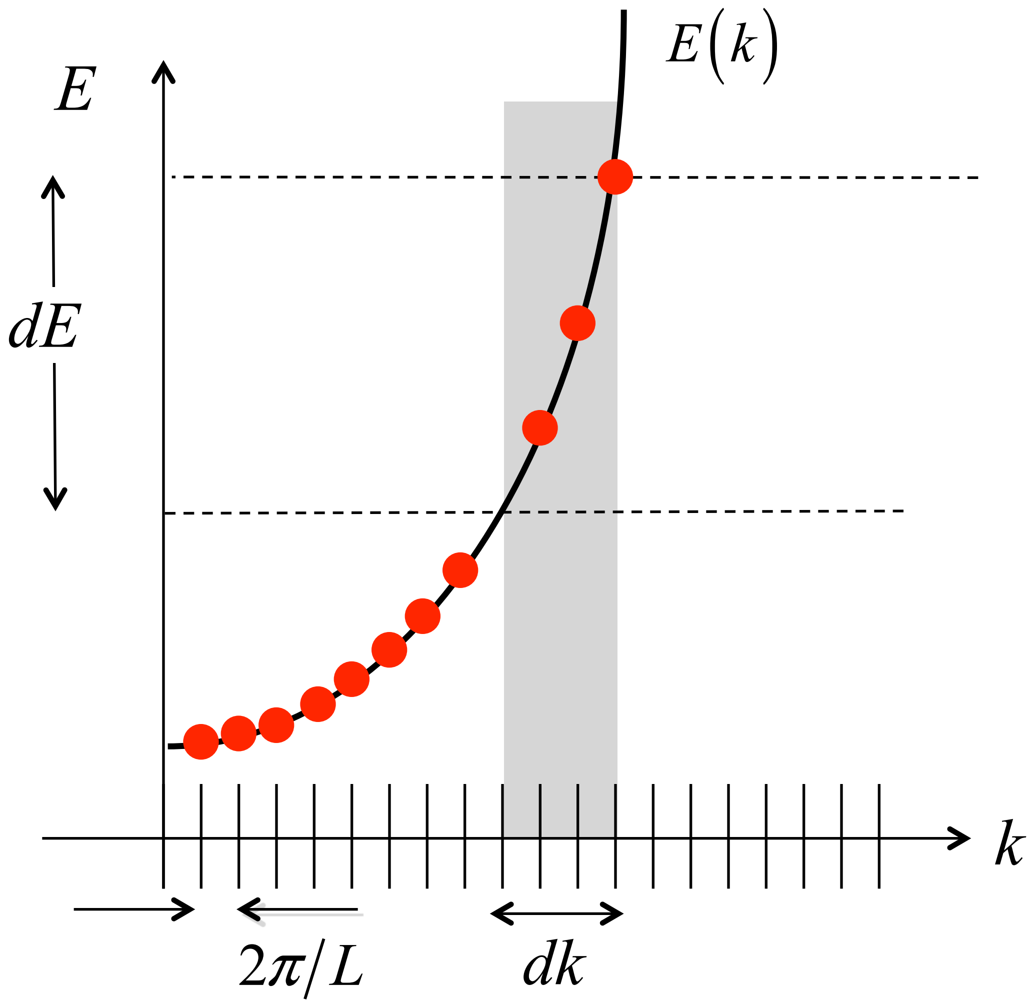


$$E'\left(1+\alpha E'\right)=\frac{\hbar^2 k^2}{2m^*(0)}$$

$$E' = E - \varepsilon_1$$

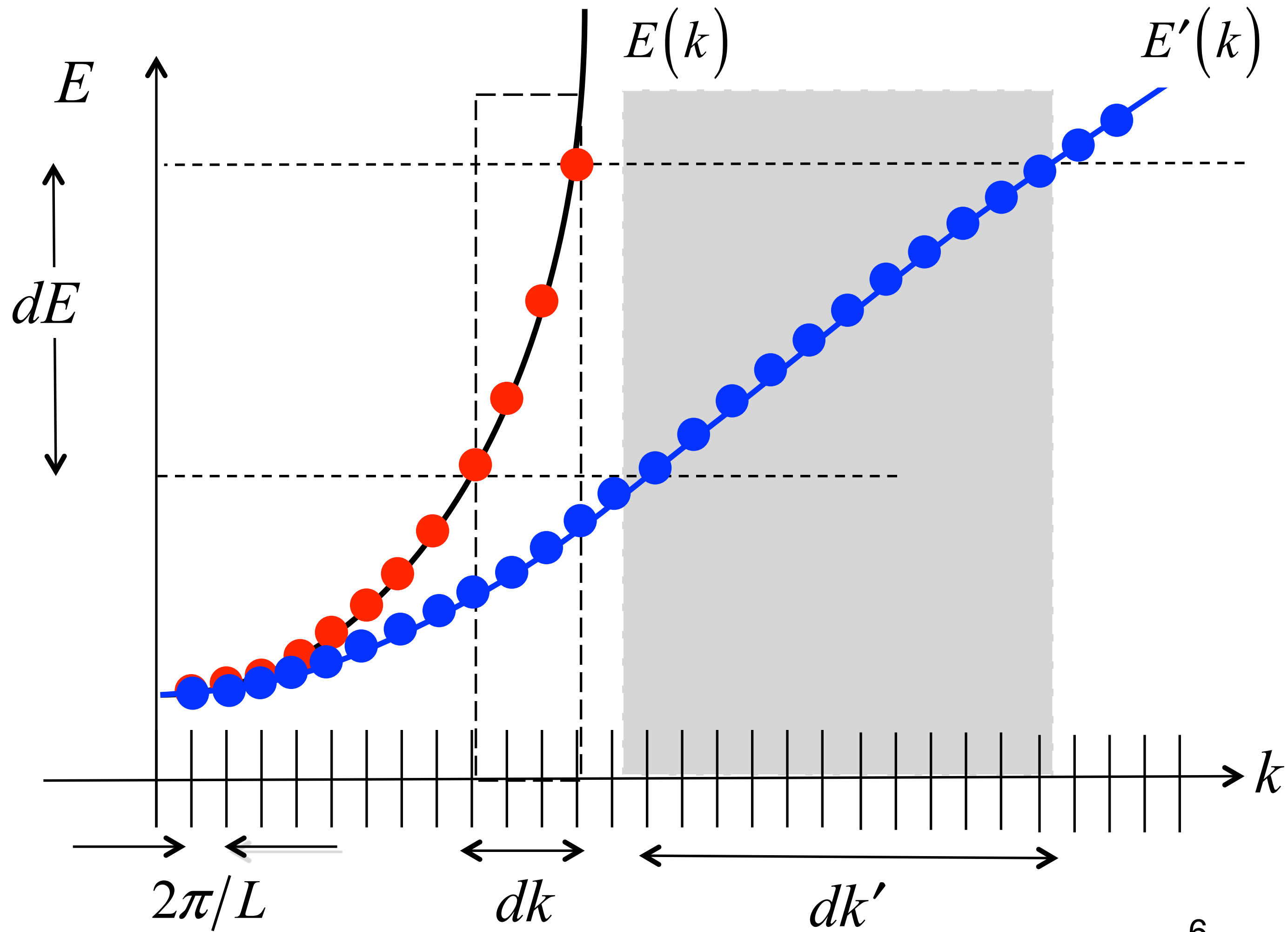
effect on DOS

How many states in this range of energies?

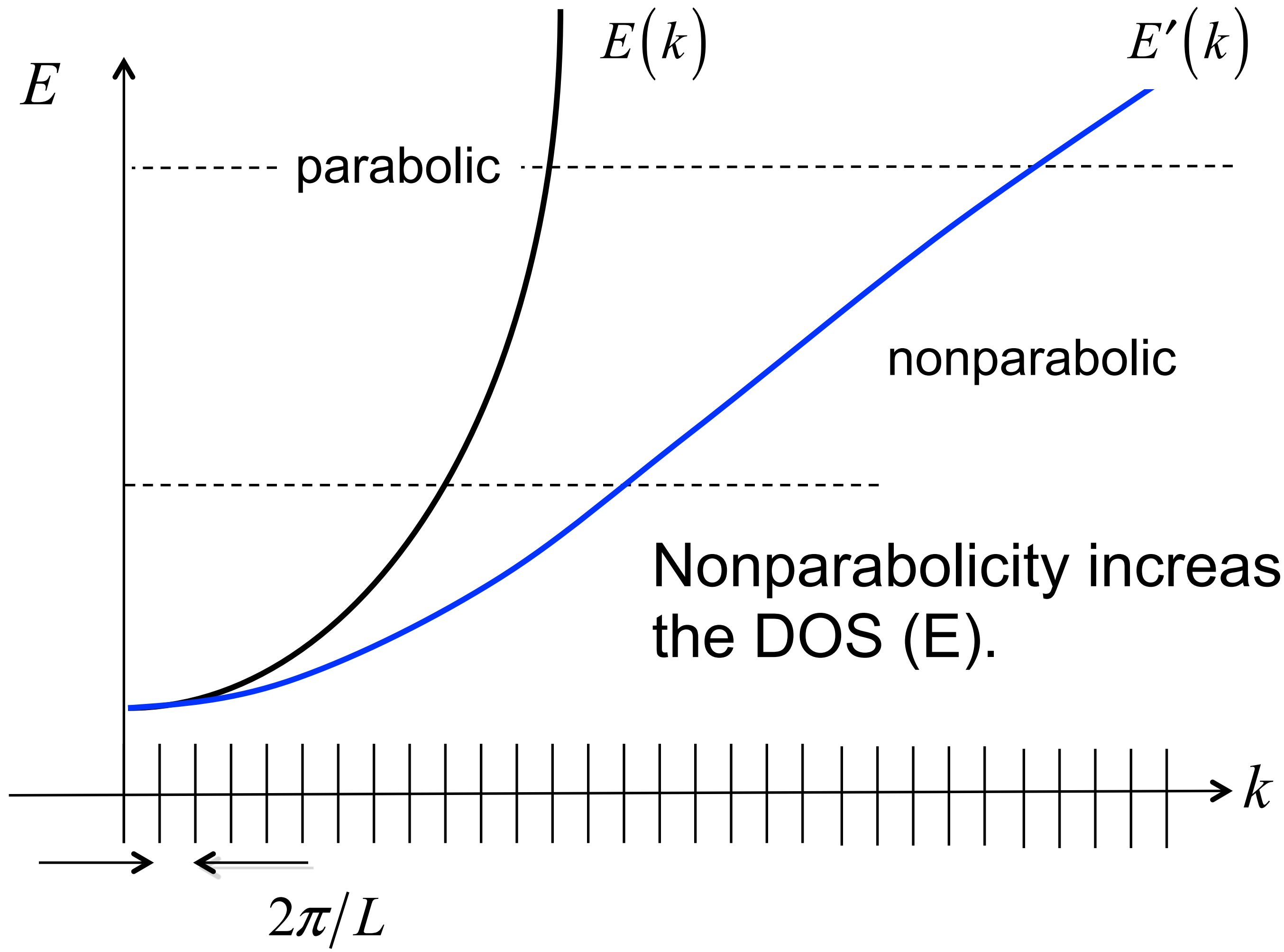


effect on DOS

How many states in this range of energies?



effect on DOS

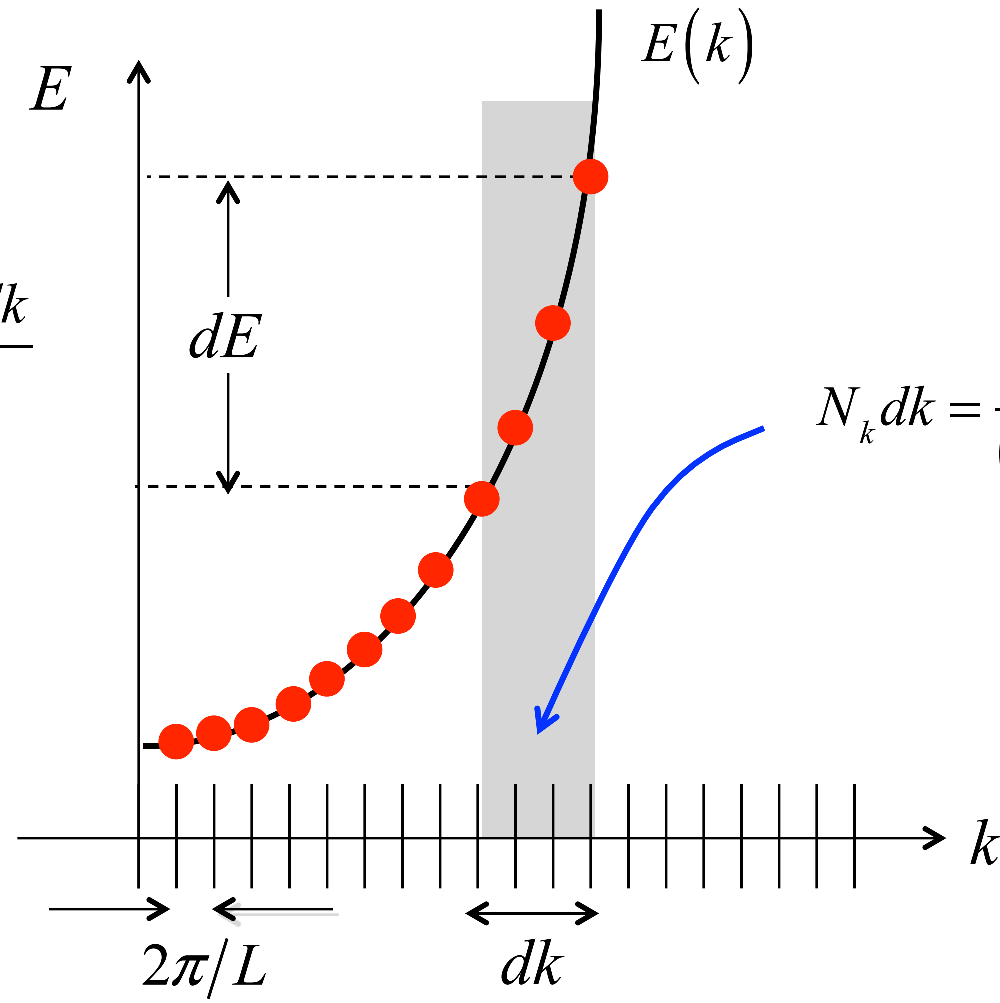


Nonparabolicity increases the DOS (E).

Example: 1D

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

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



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

1D DOS

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

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

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

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

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

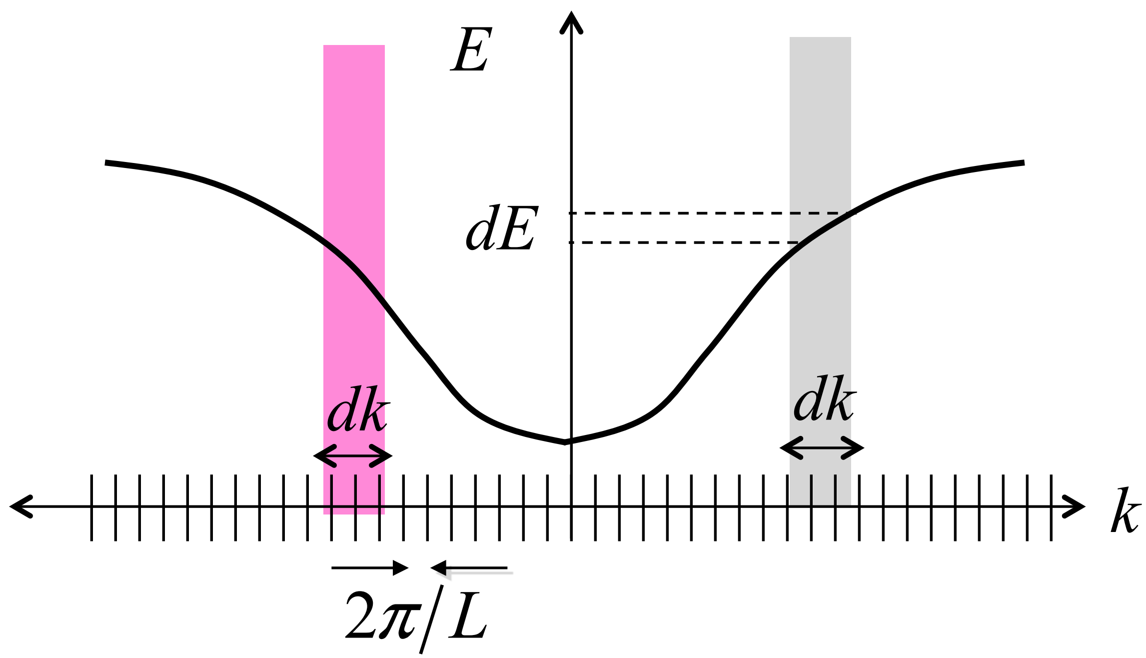
$$N_k dk = \frac{dk}{(2\pi/L)} \times 2$$

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

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

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

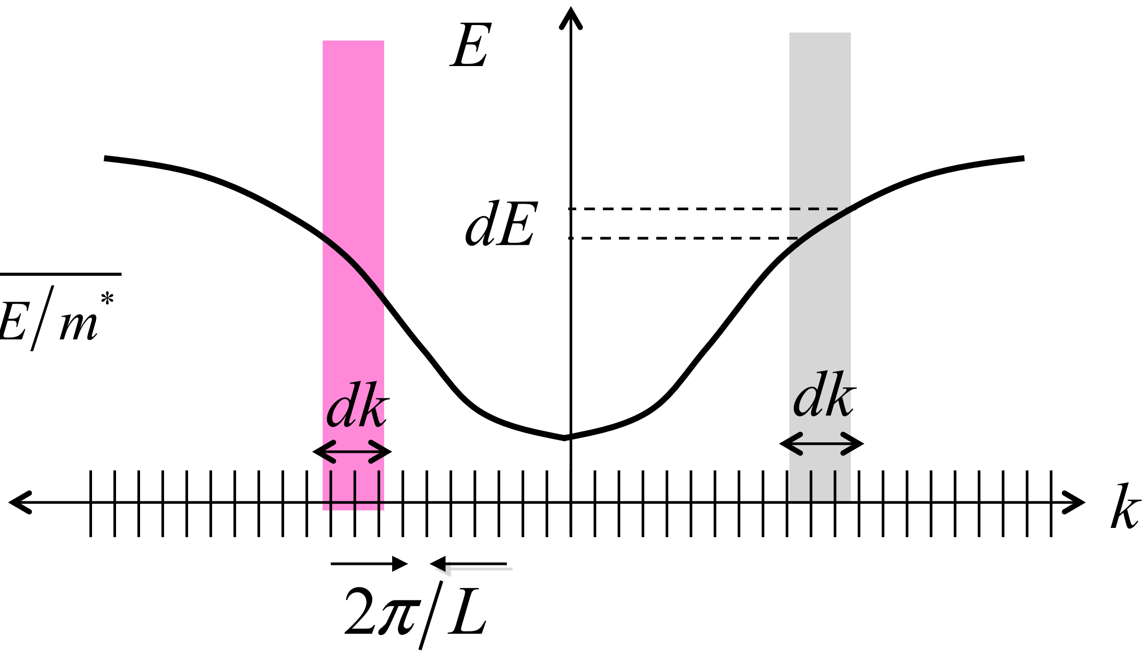
1D DOS



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

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

1D DOS



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

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

alternative expression for DOS

$$D_{1D}(E)dE = \frac{1}{L}\sum_{k}\Delta_{E,E_k}$$

$$D_{2D}(E)dE = \frac{1}{A}\sum_{\vec{k}}\Delta_{E,E_k}$$

like a "Kronecker delta"

$$D_{3D}(E) = \frac{1}{\Omega}\sum_{\vec{k}}\Delta_{E,E_k}$$

one if: $E - dE/2 < E_k < E + dE/2$

otherwise zero

example: 2D DOS for parabolic energy bands

$$D_{2D}(E_1) = \frac{1}{A}\sum_{\vec{k}} \Delta_{E',E_k}$$

$$D_{2D}(E_1) = \frac{1}{A}\sum_{\vec{k}} \delta_{E_1,E_k} \rightarrow \frac{1}{A} g_V \frac{A}{(2\pi)^2} \times 2\int_0^\infty 2\pi k\, dk\, \delta\left(E_1 - E(k)\right)$$

$$D_{2D}(E_1) = g_V \frac{1}{\pi} \times \int_0^\infty k\, dk\, \delta\left(E_1 - E(k)\right)$$

$$E(k) = \frac{\hbar^2 k^2}{2m^*} \qquad dE = \frac{\hbar^2 2k dk}{2m^*} \qquad kdk = \frac{m^*}{\hbar^2} dE$$

$$D_{2D}(E_1) = g_V \frac{m^*}{\pi\hbar^2} \times \int_0^\infty dE\, \delta\left(E_1 - E(k)\right)$$

example: 2D DOS for parabolic energy bands

$$D_{2D}(E_1) = \frac{1}{A}\sum_{\vec{k}} \Delta_{E_1,E_k} = g_V \frac{m^*}{\pi\hbar^2} \quad ✓$$

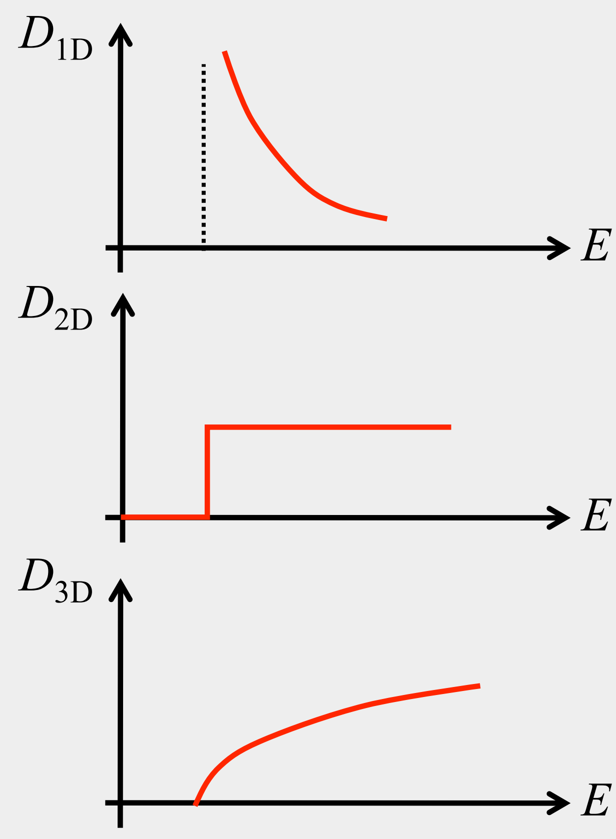
parabolic bands: 1D, 2D, and 3D

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

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

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

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



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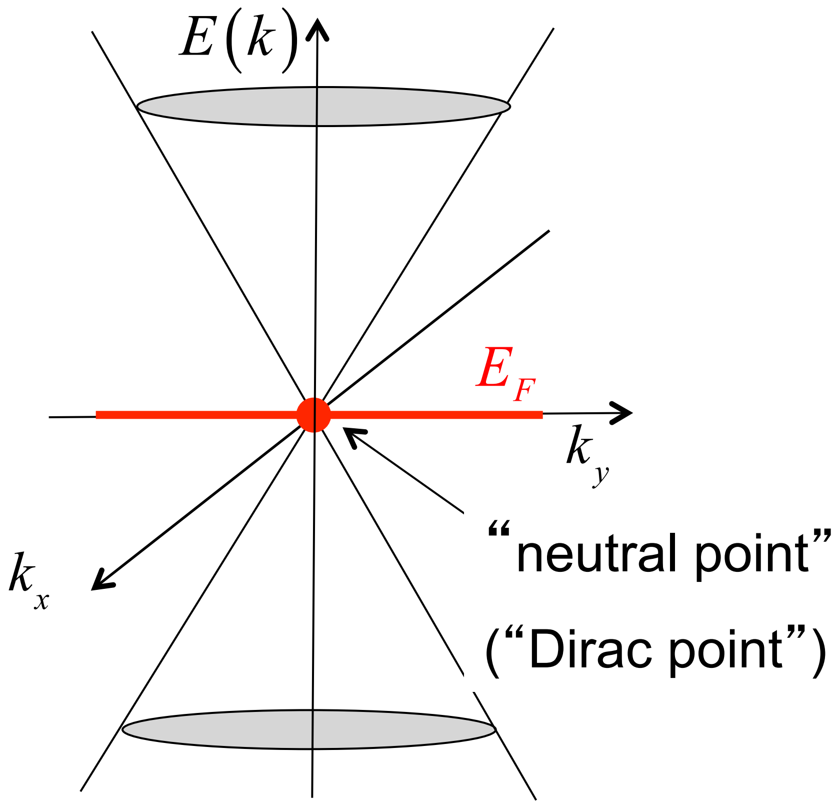
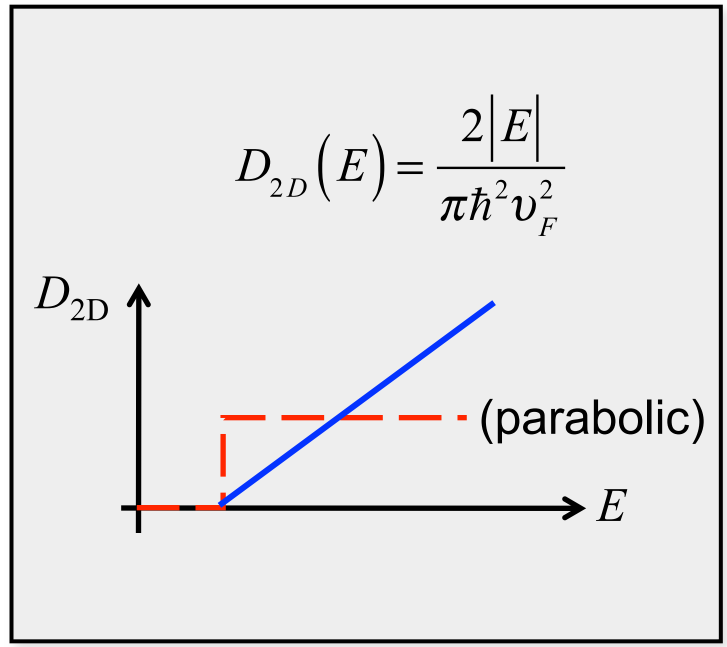
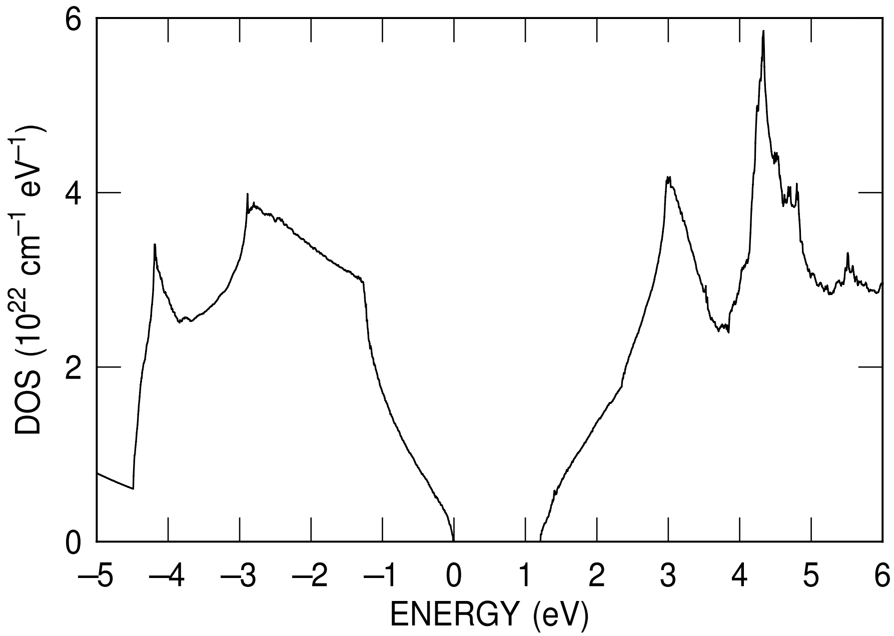
graphene (2D)



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



DOS for bulk Si



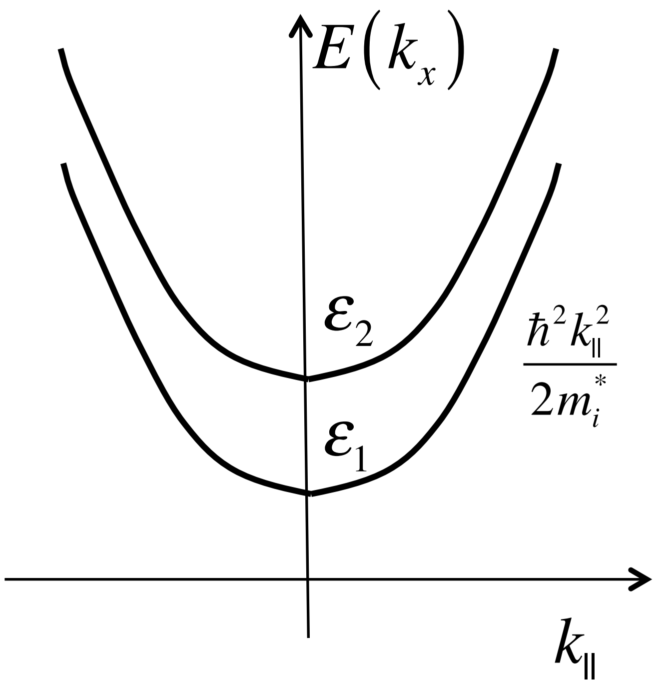
$$D_{3D}(E_1) = \frac{1}{\Omega} \sum_{\vec{k}} \Delta_{E_1, E_{\vec{k}}}$$

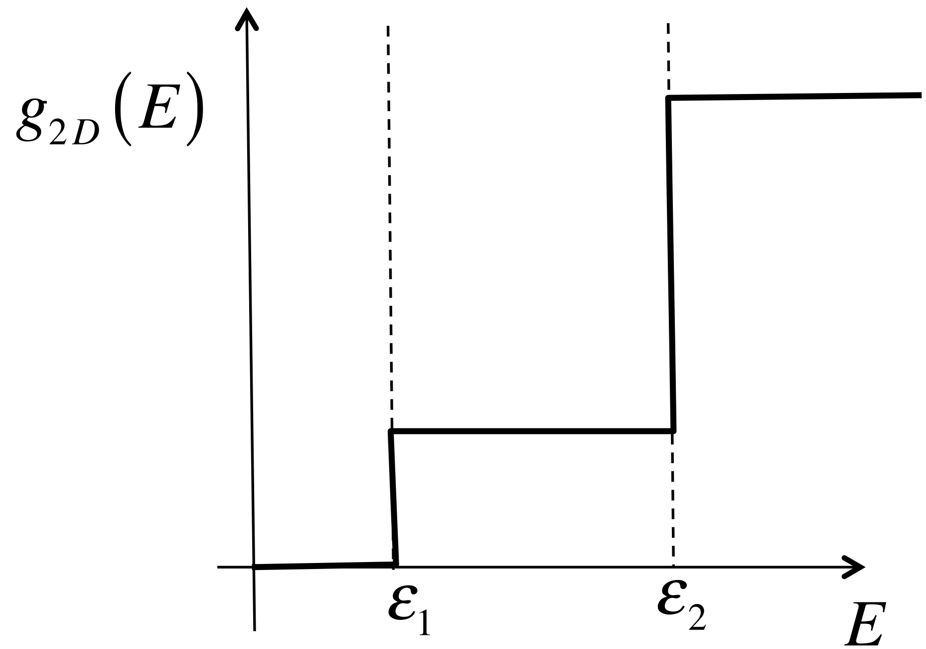
The DOS is calculated with nonlocal empirical pseudopotentials including the spin-orbit interaction.
(Courtesy Massimo Fischetti, August, 2011.)

DOS for a Si quantum well

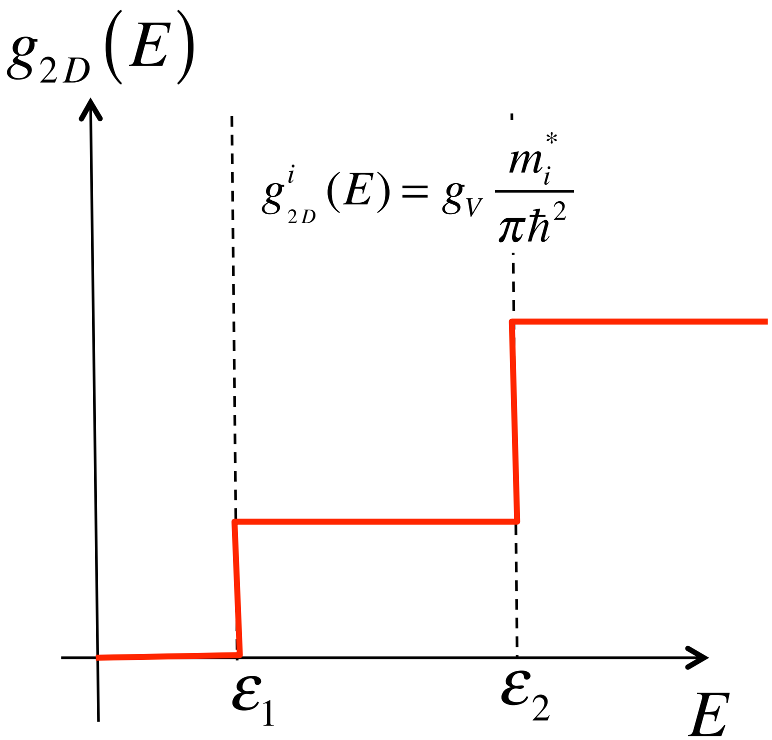
$$E = \varepsilon_i + \frac{\hbar^2 k_\parallel^2}{2m_i^*}$$

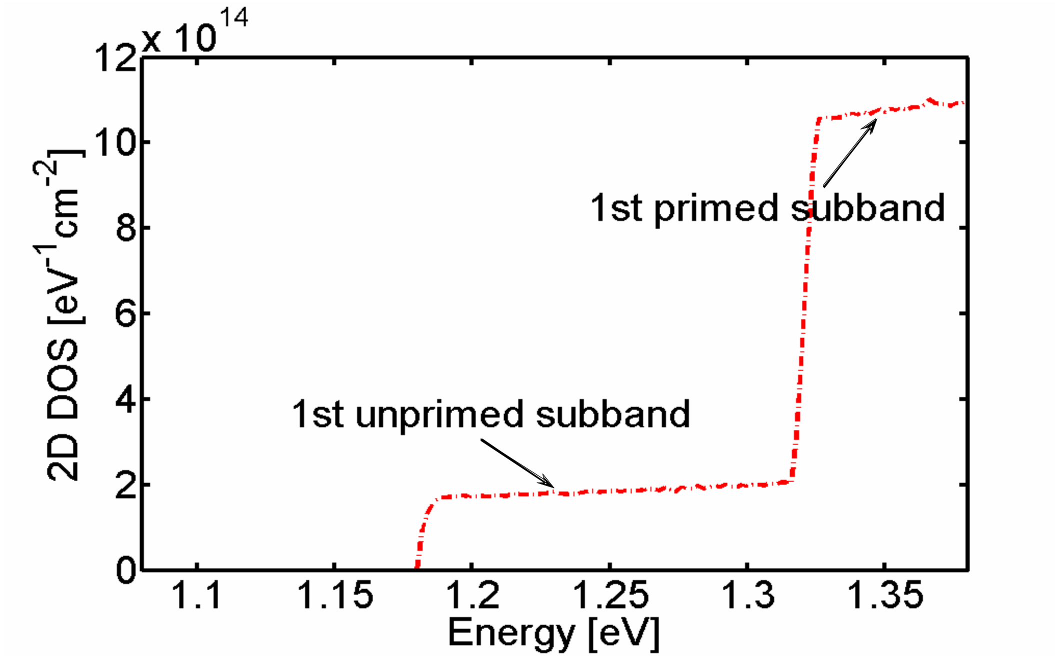
$$g_{2D}^i(E) = g_V \frac{m_i^*}{\pi\hbar^2}$$





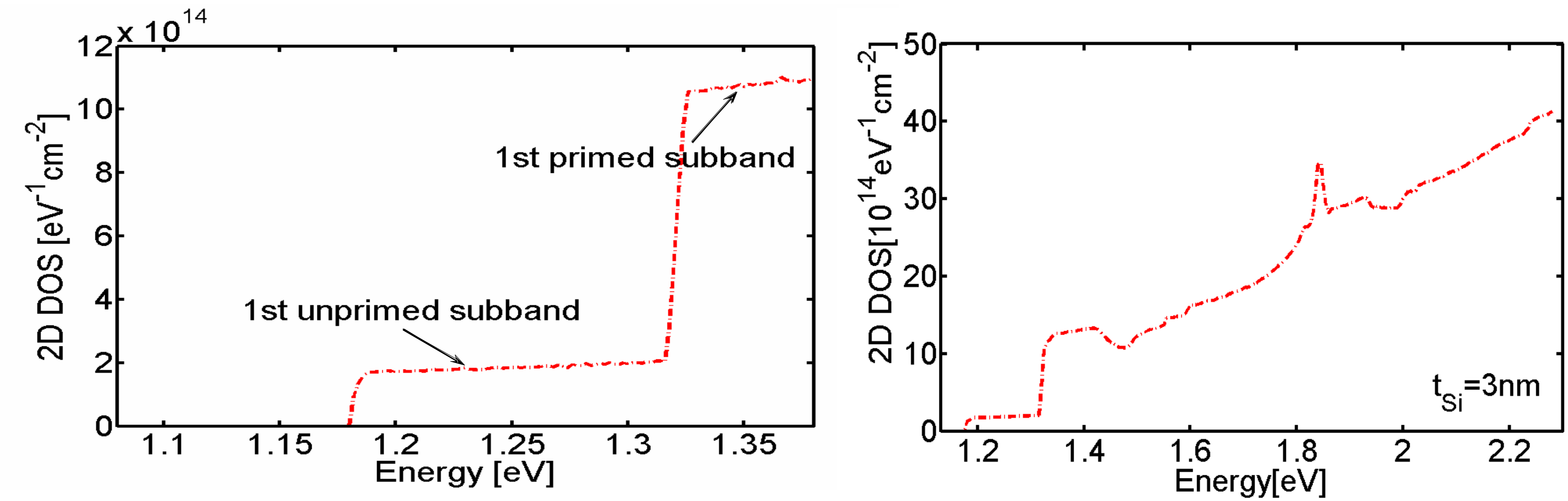
DOS for a Si quantum well





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

DOS for a Si quantum well



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

summary

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

2) The DOS becomes complicated at high energies.