ECE-656: Fall 2009

Lecture 4: Density of States/ Density of Modes

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Datta-Landauer Approach

$$I = \frac{2q}{h}\int \gamma\, \pi \frac{D(E)}{2}\left(f_1 - f_2\right) dE$$

$$I = \frac{2q}{h}\int T(E) M(E)\left(f_1 - f_2\right) dE$$

Key parameters:

1) Density-of-states (for carrier density)
2) Density of modes (for current)
3) Transmission (to describe scattering)

k-space vs. energy-space

$$N(k)\,d^3k = \frac{\Omega}{4\pi^3}\,d^3k = D(E)\,dE$$

N(*k*): independent of bandstructure

D(E): depends on *E*(*k*)

N(*k*) and *D*(*E*) are proportional to the volume, *Ω*, but it is common to express *D*(*E*) per unit energy and per unit volume. We will use the **same symbol** in both cases, but the units will be clear from the context.

outline

1) **Density of states**

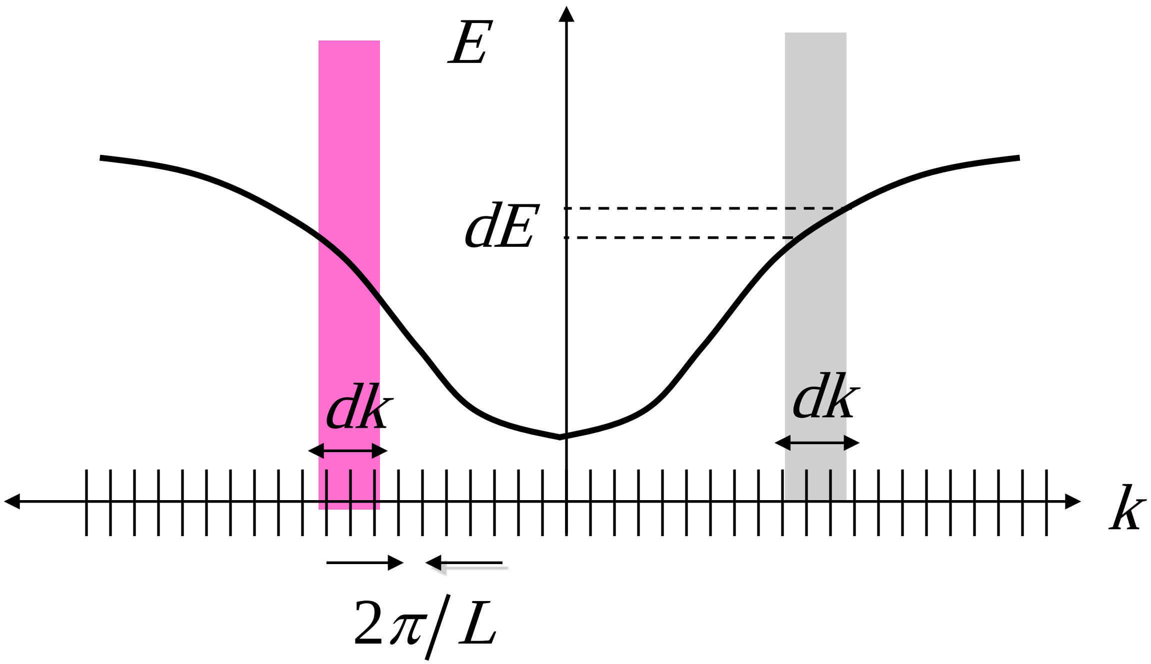
2) Example: graphene

3) Density of modes

4) Example: graphene

5) Summary

example: 1D DOS



$$N_{1D}(k)dk = \left(\frac{L}{2\pi} \times 2\right) dk$$

$$D_{1D}^{+}(E)dE = N_{1D}(k)dk / L$$

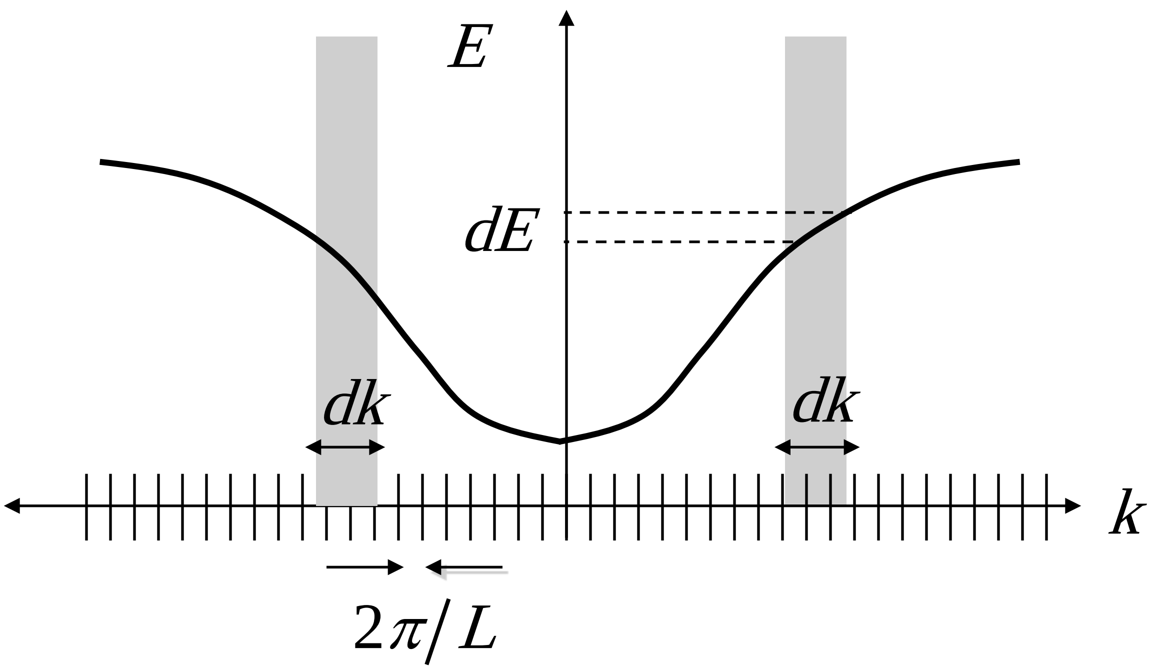
$$D_{1D}^{+}(E)dE = \frac{1}{\pi} dk$$

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

$$\upsilon(k) = \frac{1}{\hbar}\frac{dE}{dk}$$

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

example: 1D DOS for parabolic bands



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

independent of *E*(*k*)

parabolic E(*k*)

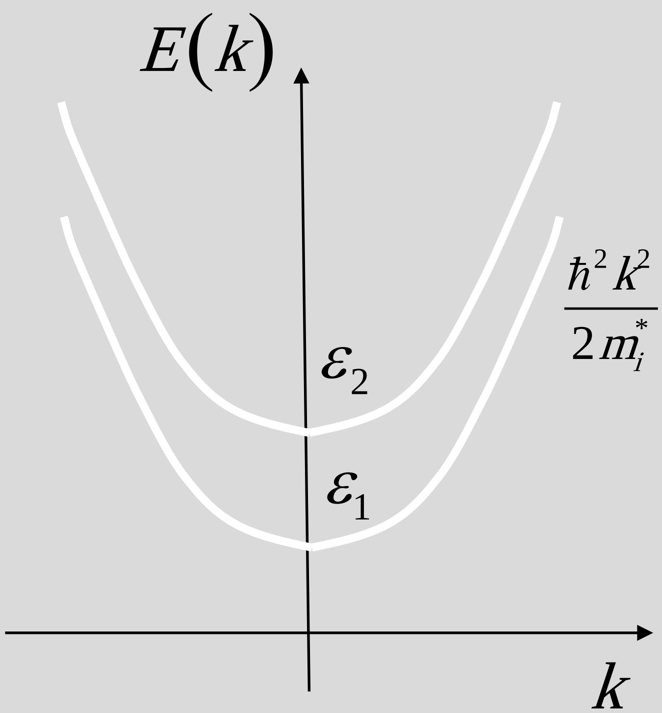
$$E(k) = \frac{\hbar^2 k^2}{2m^*}$$

$$\frac{1}{\hbar}\frac{dE}{dk} = \upsilon = \sqrt{\frac{2E}{m^*}}$$

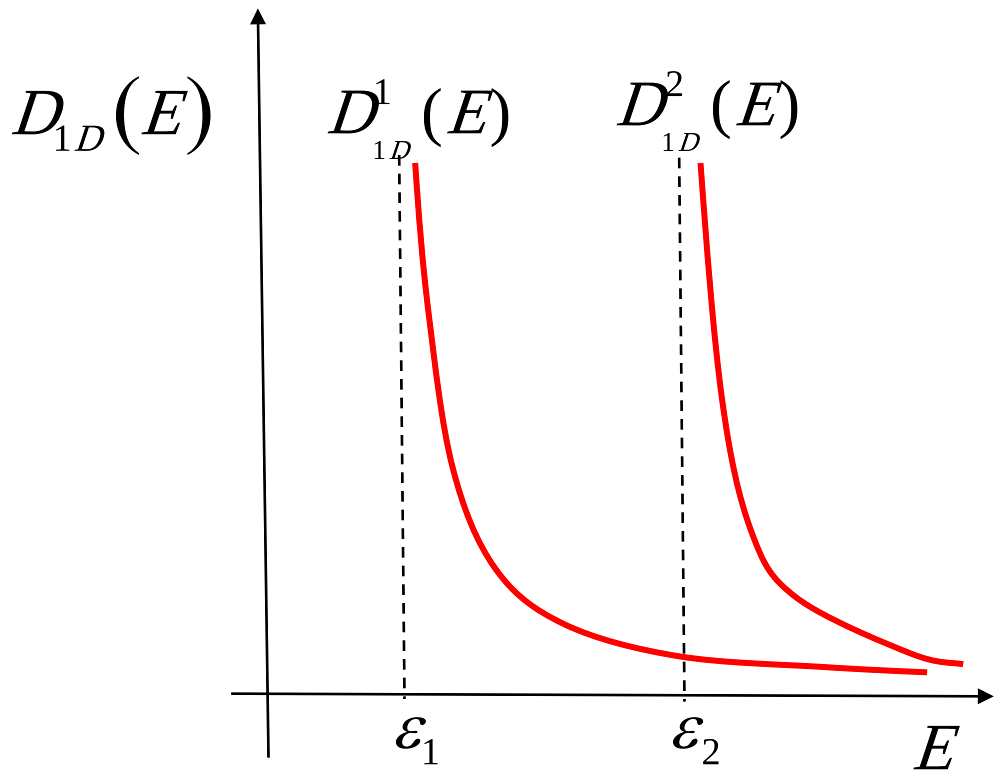
$$D_{1D}(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m^*}{E}}$$

density of states in a nanowire

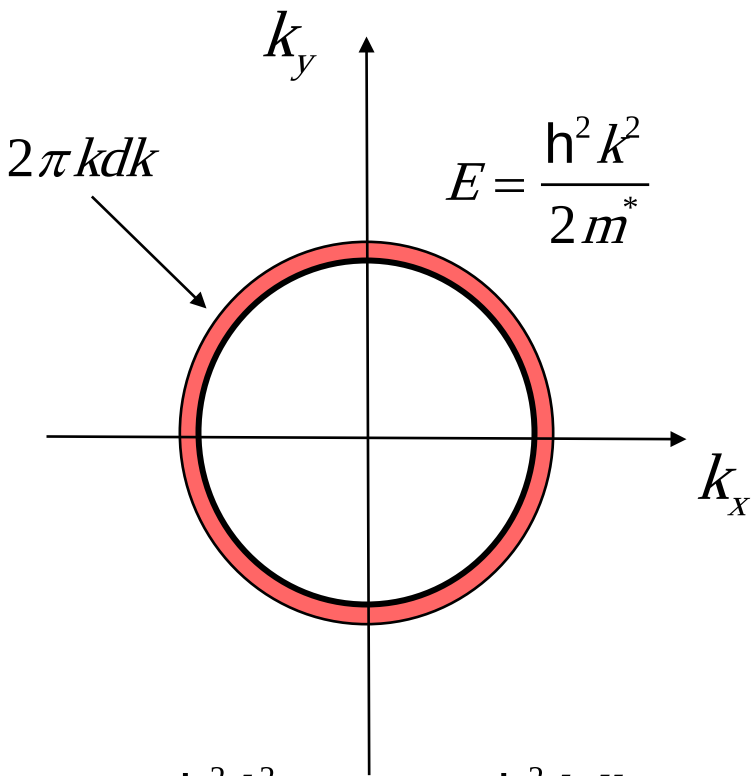
$$E = \varepsilon_i + \frac{\hbar^2 k^2}{2 m_i^*}$$



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



2D density of states



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

$$N_{2D}(k)dk = \left(\frac{A}{(2\pi)^2} \times 2\right) dk_x dk_y$$

$$D_{2D}(E)dE = N_{2D}(k) 2\pi kdk / A$$

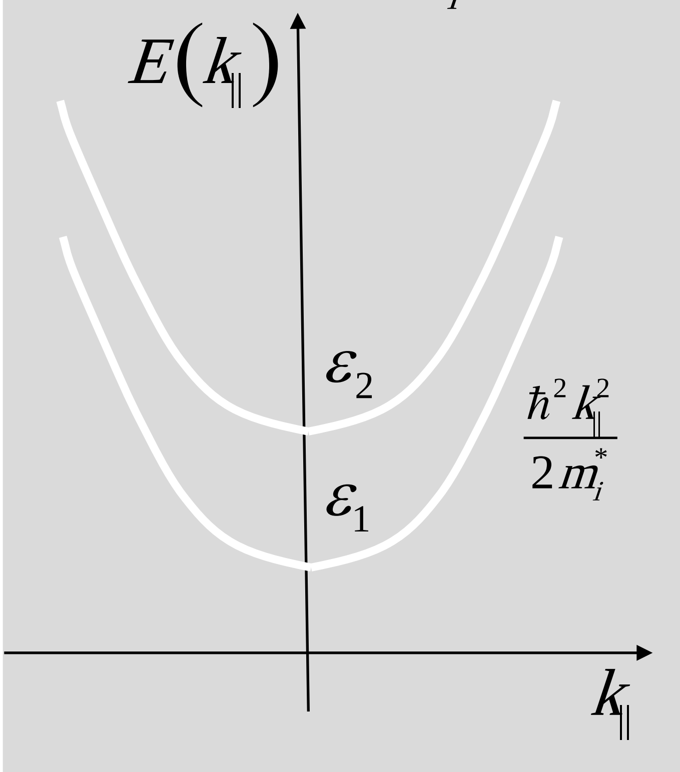
$$D_{2D}(E)dE = \frac{1}{2\pi^2} 2\pi kdk$$

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

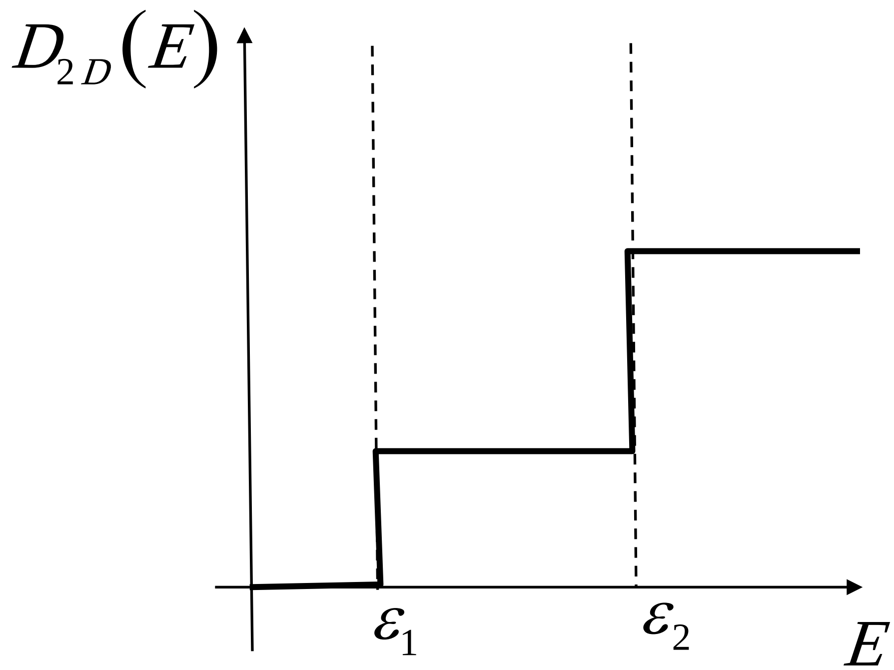
$$D_{2D}(E) = \frac{m^*}{\pi\hbar^2}$$

density of states in a film

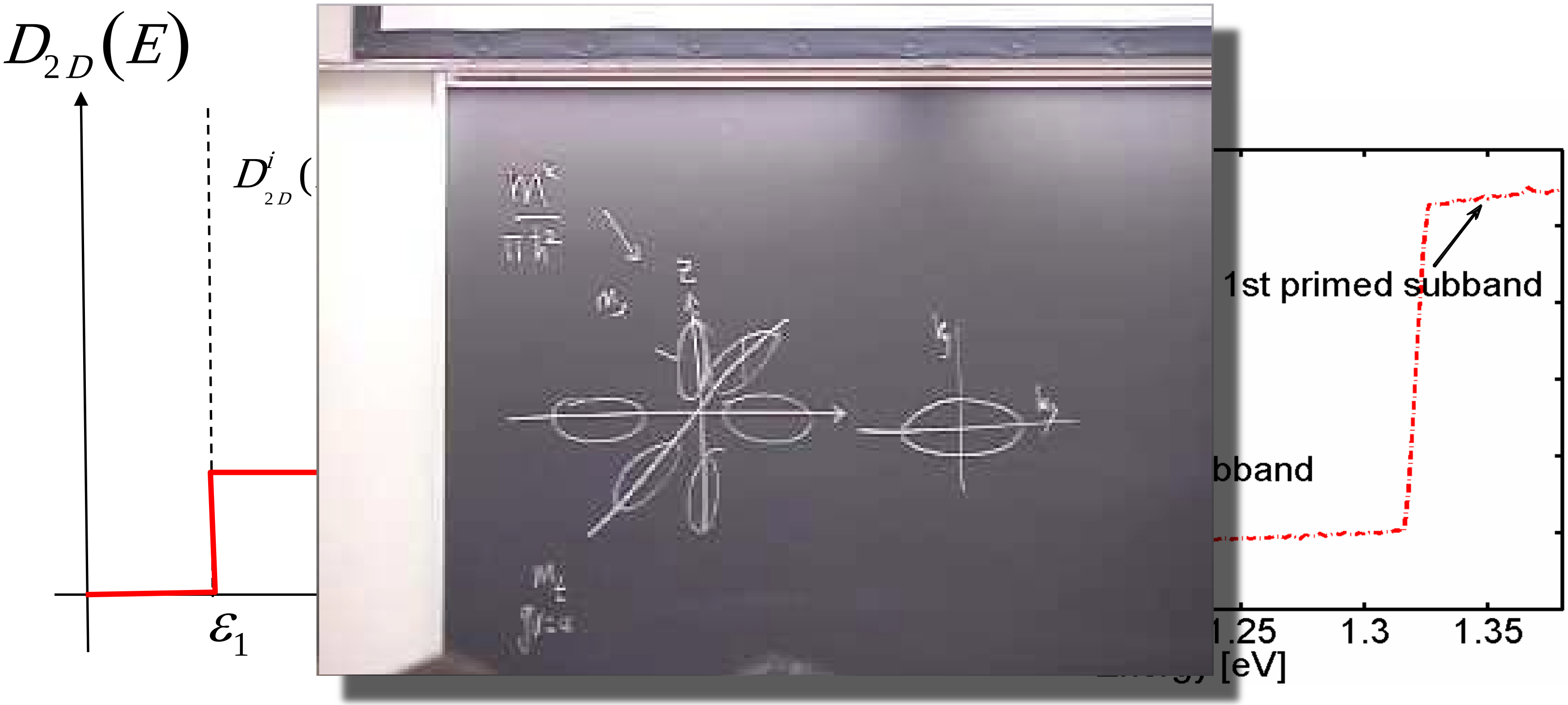
$$E = \varepsilon_i + \frac{\hbar^2 k_\parallel^2}{2 m_i^*}$$



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



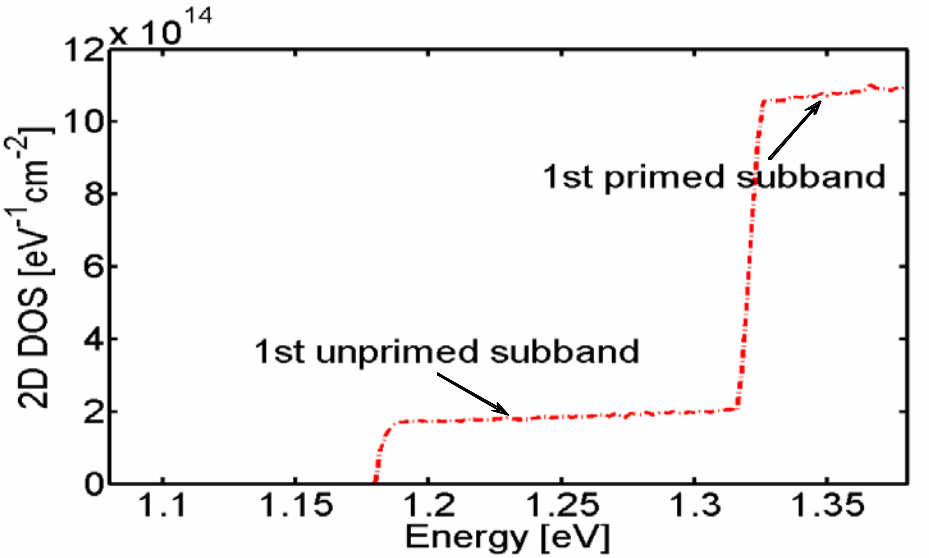
effective mass vs. tight binding



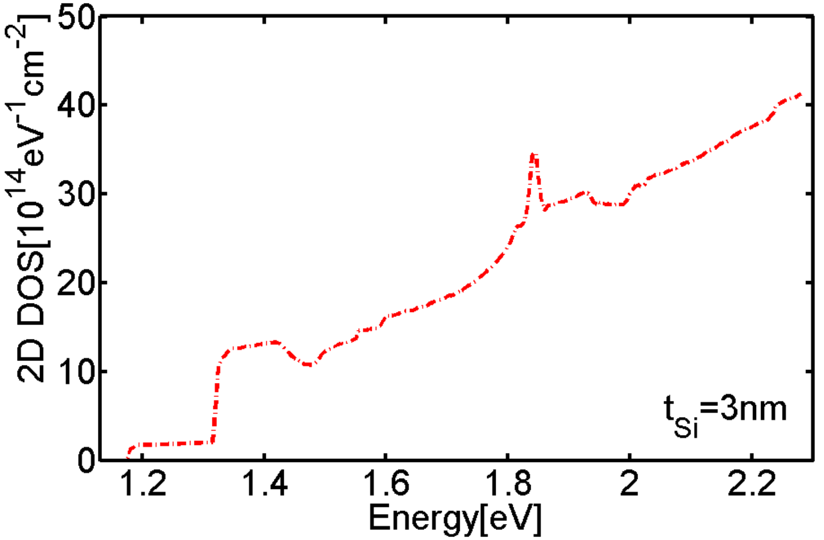
sp^{3}s*d^5 tight binding calculation by
Yang Liu, Purdue University, 2007

effective mass vs. tight binding

near subband edge

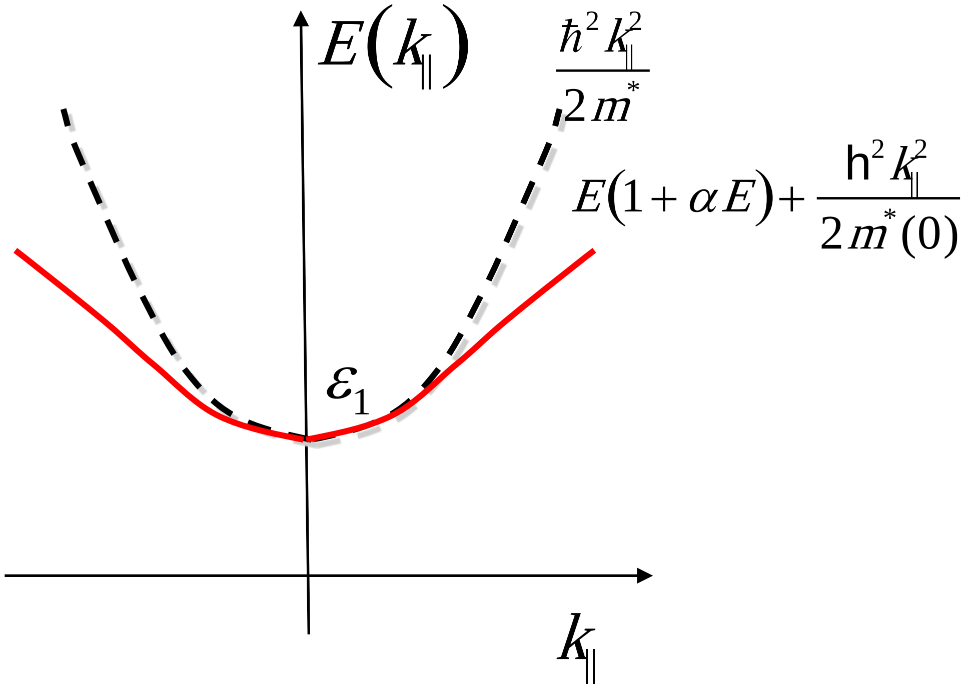


well above subband edge



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

exercise



$$E = \varepsilon_1 + E(k_{\parallel})$$

$$E_k(1+\alpha E_k)+\frac{\hbar^2 k_{\parallel}^2}{2m^*(0)}$$

$$D_{2D} = ?$$

alternative approach

$$D_{1D}(E) = \frac{1}{L}\sum_{k}\delta\left(E - E_k\right)$$

$$D_{2D}(E) = \frac{1}{A}\sum_{\mathbf{k}}\delta\left(E - E_{\mathbf{k}}\right)$$

$$D_{3D}(E) = \frac{1}{\Omega}\sum_{\mathbf{k}}\delta\left(E - E_{\mathbf{k}}\right)$$

proof

in k-space, we know:

$$n_L = \frac{1}{L}\sum_k f_0(E_k)$$

can also work in energy-space:

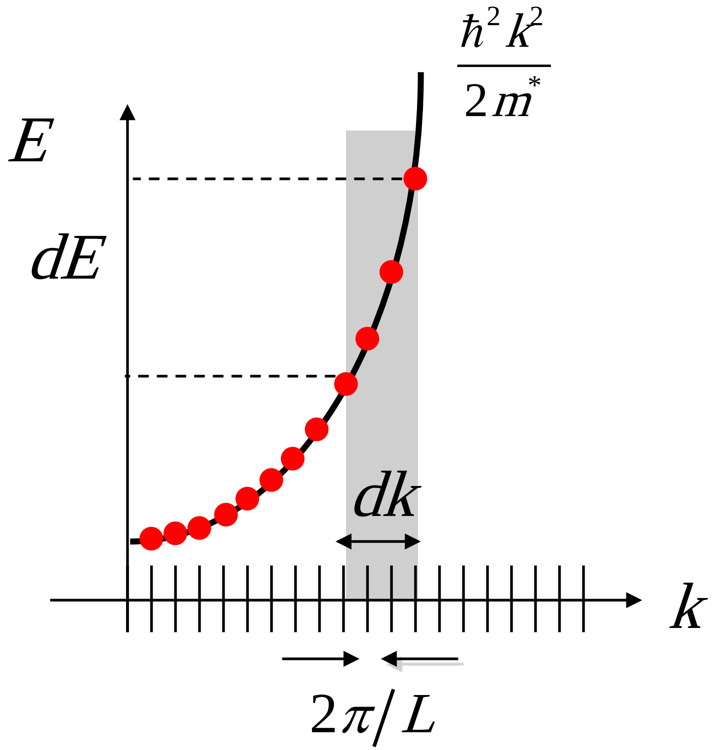
$$n_L = \int f_0(E) D_{1D}(E) dE$$

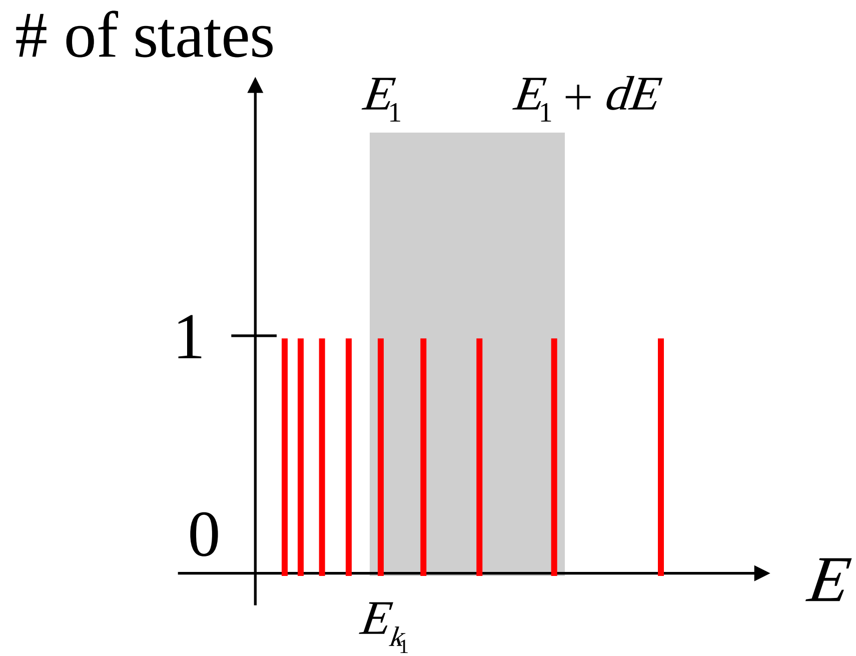
$$n_L = \int f_0(E) \frac{1}{L}\sum_k \delta(E - E_k) dE$$

$$n_L = \frac{1}{L}\sum_k \int f_0(E) \delta(E - E_k) dE$$

$$n_L = \frac{1}{L}\sum_k f_0(E_k)$$

interpretation





$$\int_{E_1}^{E_1+dE} D_{1D}(E)\,dE = \int_{E_1}^{E_1+dE} \frac{1}{L}\sum_k \delta\left(E - E_k\right)dE = \frac{1}{L}\sum_k \int_{E_1}^{E_1+dE} \delta\left(E - E_k\right)dE$$

counts the states between E and E +dE

outline

1) Density of states

2) **Example: graphene**

3) Density of modes

4) Example: graphene

5) Summary

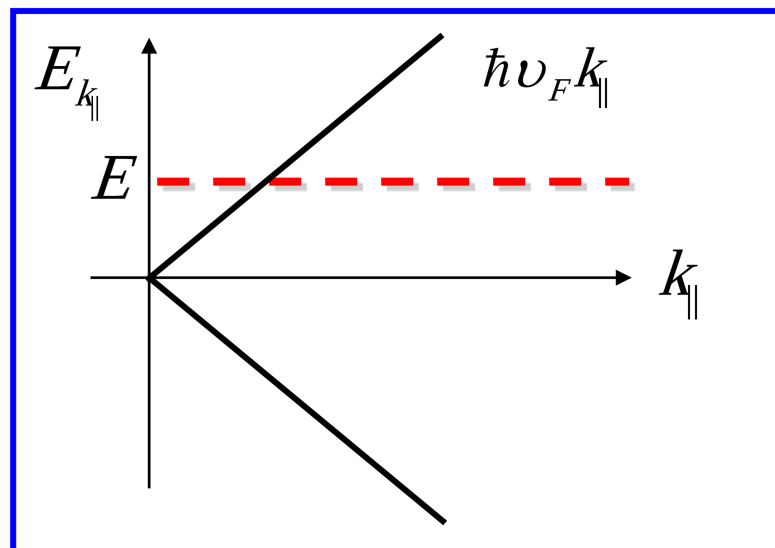
example: DOS for graphene

$$D(E) = \frac{1}{A}\sum_{k_\parallel}\delta\left(E - E_{k_\parallel}\right) = \frac{1}{A}\frac{A}{\left(2\pi^2\right)} \times 2\int_0^\infty \delta(E - E_{k_\parallel})2\pi k_\parallel \, dk_\parallel$$

$$E_{k_\parallel} = \hbar\upsilon_F k_\parallel \qquad dE_{k_\parallel} = \hbar\upsilon_F dk_\parallel \qquad k_\parallel dk_\parallel = E_{k_\parallel} dE_{k_\parallel} \big/ \hbar^2\upsilon_F^2$$

$$D(E) = \frac{g_V}{\pi\hbar^2\upsilon_F^2}\int_0^\infty \delta(E - E_{k_\parallel})E_{k_\parallel} \, dE_{k_\parallel}$$

$$D(E) = \frac{2E}{\pi\hbar^2\upsilon_F^2} \qquad E > 0$$



outline

1) Density of states

2) Example: graphene

3) **Density of modes**

4) Example: graphene

5) Summary

definitions

$$I = \left\{ \frac{2q^2}{h} \int T(E) M(E) \left(-\partial f_0 / \partial E \right) dE \right\} V$$

(near-equilibrium)

$$M(E) = \gamma \pi \frac{D(E)}{2} \qquad \gamma(E) = \frac{\hbar}{\tau(E)}$$

$$T(E) = \frac{\lambda(E)}{\lambda(E) + L}$$

DOS vs. DOM

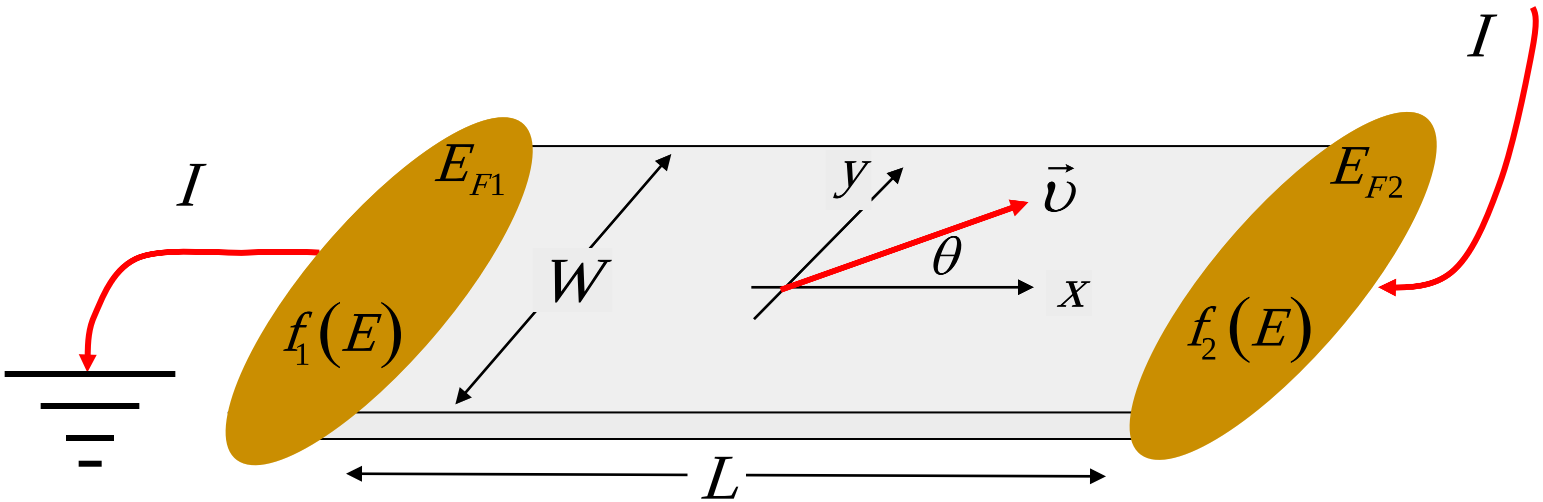
$$N = \int D(E)\, f_0(E)\, dE$$

$$G = \int M(E)\left(-\partial f_0 / \partial E\right) dE \qquad \left(T(E) = 1\right)$$

Density of states determines the carrier density and density of modes determines the conductance.

$$\begin{aligned}
&\text{1D}: \quad D(E) \propto L \quad M(E) \propto 1 \\
&\text{2D}: \quad D(E) \propto A \quad M(E) \propto W \\
&\text{3D}: \quad D(E) \propto \Omega \quad M(E) \propto A
\end{aligned}$$

modes (conducting channels) in 2D



$$M_{2D}(E) = \gamma \pi D_{2D}(E)/2 = ?$$

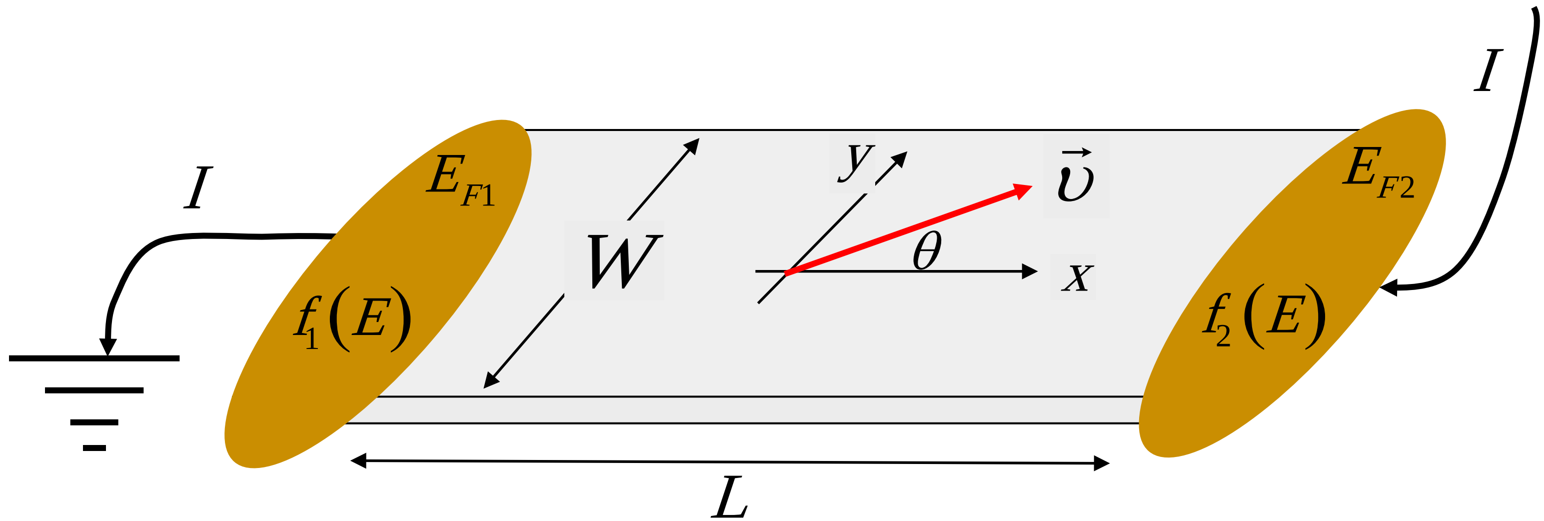
$$\psi(x,y) \propto e^{ik_x x} \sin k_y y$$

We will assume that *W* is wide (small *W*, is a '1D' nanowire).

$$k_y = m\pi/W \quad m = 1, 2, \ldots$$

$$\tan\theta = k_y/k_x$$

modes (conducting channels) in 2D



$M_{2D}(E) = \gamma\,\pi\,D_{2D}(E)/2$ $\quad D_{2D}(E) = A\left(m^*/\pi h^2\right)$ $\quad \left(E(k) = h^2k^2/2m^*\right)$

$$\gamma = h/\langle\tau\rangle$$

$$\langle\cos\theta\rangle = \frac{\int_{-\pi/2}^{+\pi/2}\cos\theta\, d\theta}{\pi}$$

$$\gamma = \frac{h\upsilon}{L}\left(\frac{2}{\pi}\right)$$

$$\gamma = \frac{h}{L/\langle\upsilon_x\rangle} = \frac{h\upsilon}{L}\langle\cos\theta\rangle$$

$$\langle\cos\theta\rangle = \frac{2}{\pi}$$

$$\upsilon = \sqrt{\frac{2(E-\varepsilon_1)}{m^*}}$$

modes in 2D

$$M(E) = \gamma(E)\pi D_{2D}(E)/2$$

$$\gamma(E) = \frac{\hbar\upsilon}{L}\left(\frac{2}{\pi}\right) = \frac{\hbar\sqrt{2(E-\varepsilon_1)/m^*}}{L}\left(\frac{2}{\pi}\right)$$

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

$$\gamma\,\pi\,D_{2D}/2 = \left(\frac{\hbar}{L}\sqrt{\frac{2(E-\varepsilon_1)}{m^*}}\frac{2}{\pi}\right)\pi\left(\frac{m^*}{2\pi\hbar^2}WL\right)$$

But how do we interpret this result physically?

$$M_{2D}(E) = W\frac{\sqrt{2m^*(E-\varepsilon_1)}}{\pi\hbar}$$

physical interpretation

$$E(k) = \varepsilon_1 + \frac{\hbar^2 k^2}{2m^*}$$

$$k(E) = \frac{\sqrt{2m^*(E - \varepsilon_1)}}{\hbar}$$

$$k(E) = \frac{2\pi}{\lambda_B(E)}$$

$$\frac{\sqrt{2m^*(E - \varepsilon_1)}}{\pi\hbar} = \frac{1}{\left(\lambda_B(E)/2\right)}$$

But how do we interpret this result physically?

$$M_{2D}(E) = W\frac{\sqrt{2m^*(E - \varepsilon_1)}}{\pi\hbar}$$

$$M_{2D}(E) = \frac{W}{\lambda_B(E)/2}$$

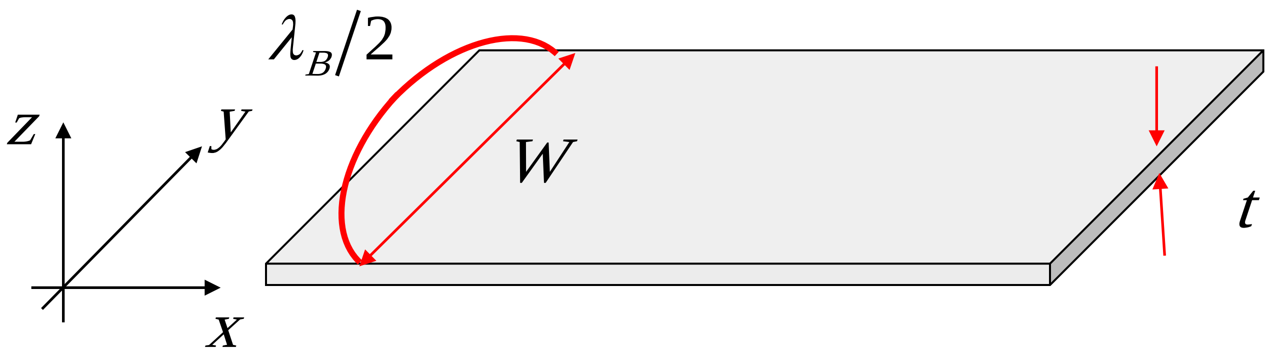
waveguide modes

Assume that there is **one** subband associated with confinement in the z-direction. **Many** subbands associated with confinement in the y-direction

$$\psi(x,y) \propto e^{ik_x x} \sin k_y y$$

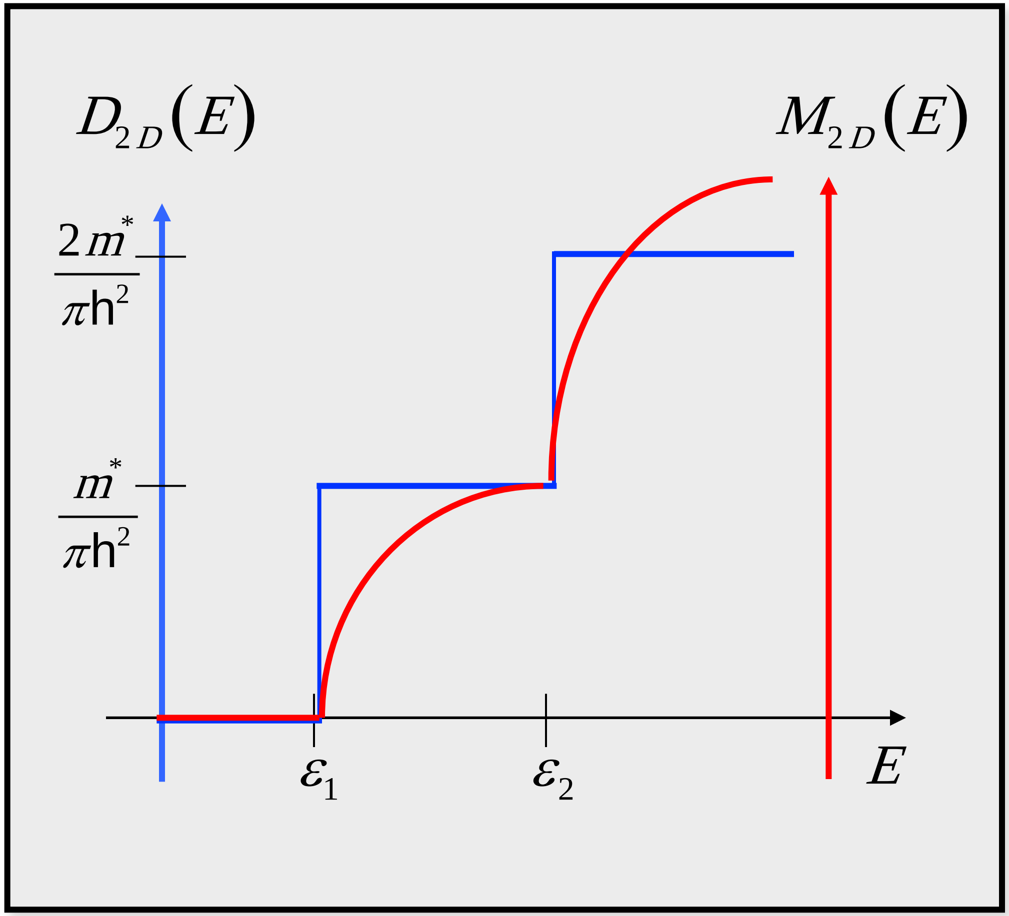
lowest mode

$$k_y = m\pi / W \quad m = 1, 2, \ldots$$



***M* = # of electron half wavelengths that fit into *W*.**

DOS vs. modes in 2D



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

$$M_{2D}(E) = \frac{W\sqrt{2m^*\left[E-\varepsilon_i(0)\right]}}{\pi\hbar}\theta(E-\varepsilon_1)$$

DOS vs. modes

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

$$M_{2D}(E) = \frac{W\sqrt{2m^*\left[E-\varepsilon_i(0)\right]}}{\pi\hbar}$$

$$\frac{M_{2D}(E)}{D_{2D}(E)} = \hbar W\sqrt{\frac{2\left[E-\varepsilon_i(0)\right]}{m^*}}$$

$$M(E) = \hbar W D_{2D}(E)\upsilon(E)$$

M(*E*) is proportional to the DOS(*E*) times velocity.

outline

1) Density of states

2) Example: graphene

3) Density of modes

4) **Example: graphene**

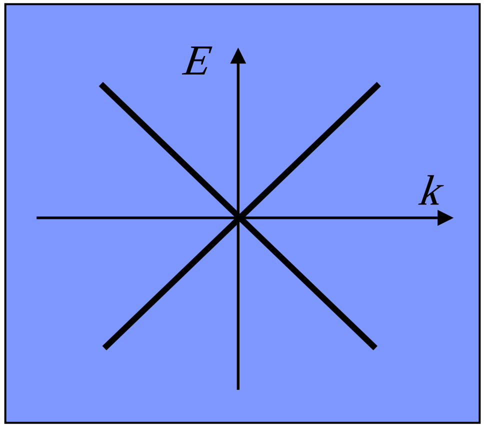
5) Summary

graphene

We have seen that $M(E)$ depends on dimensionality, but we assumed parabolic energy bands in both cases.

$$E(k) = \varepsilon_1 + \frac{\hbar^2 k^2}{2m^*}$$

But what if our 2D resistor is a sheet of graphene - with linear dispersion?



$$E(k) = \pm \hbar \upsilon_F k$$

$$\vec{k} = k_x \hat{x} + k_y \hat{y}$$

$M(E)$ for graphene

$$M(E) = \gamma(E)\pi D_{2D}(E)/2$$

$$\gamma(E) = \frac{\hbar\upsilon}{L}\left(\frac{2}{\pi}\right) = \frac{\hbar\upsilon_F}{L}\left(\frac{2}{\pi}\right)$$

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

$$\gamma\,\pi\,D_{2D}/2 = \left(\frac{\hbar\upsilon_F}{L}\frac{2}{\pi}\right)\pi\left(\frac{E}{\pi\hbar^2\upsilon_F^2}WL\right)$$

$$M(E) = \frac{2E}{\pi\hbar\upsilon_F} = 2 \times \frac{W}{\lambda_B/2}$$

- still proportional to *W*
- *proportional to E, not sqrt(E)*
- *factor of two is for valley degeneracy*

M depends on dimensionality and on the E(k).

outline

1) Density of states

2) Example: graphene

3) Density of modes

4) Example: graphene

5) **Summary**

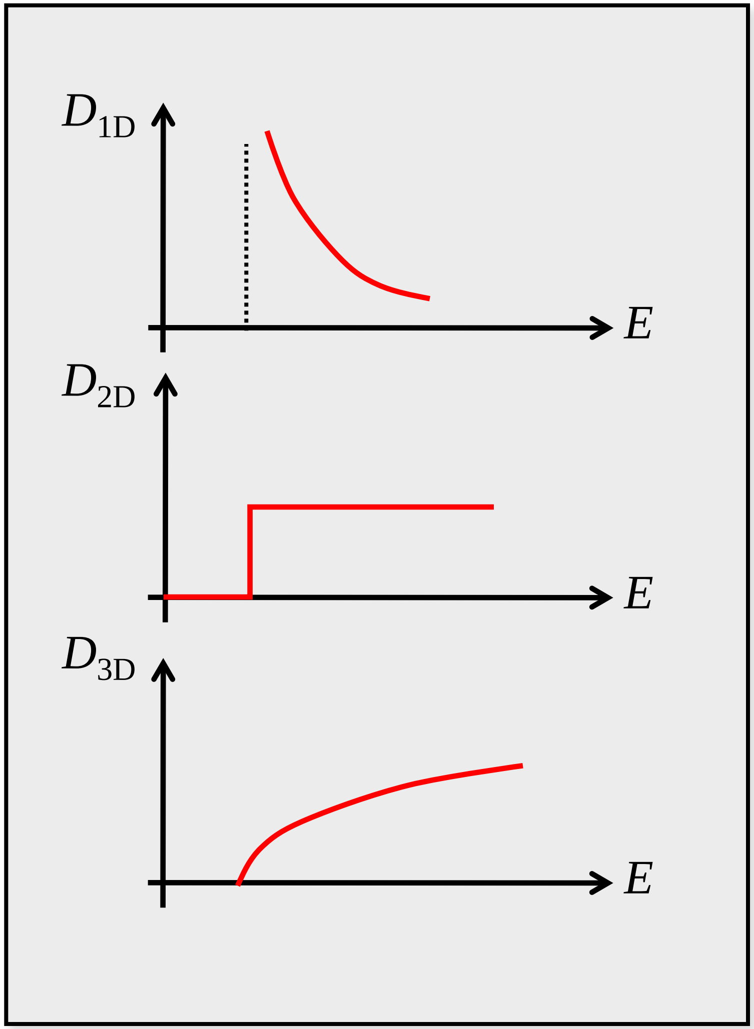
density of states

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

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

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

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



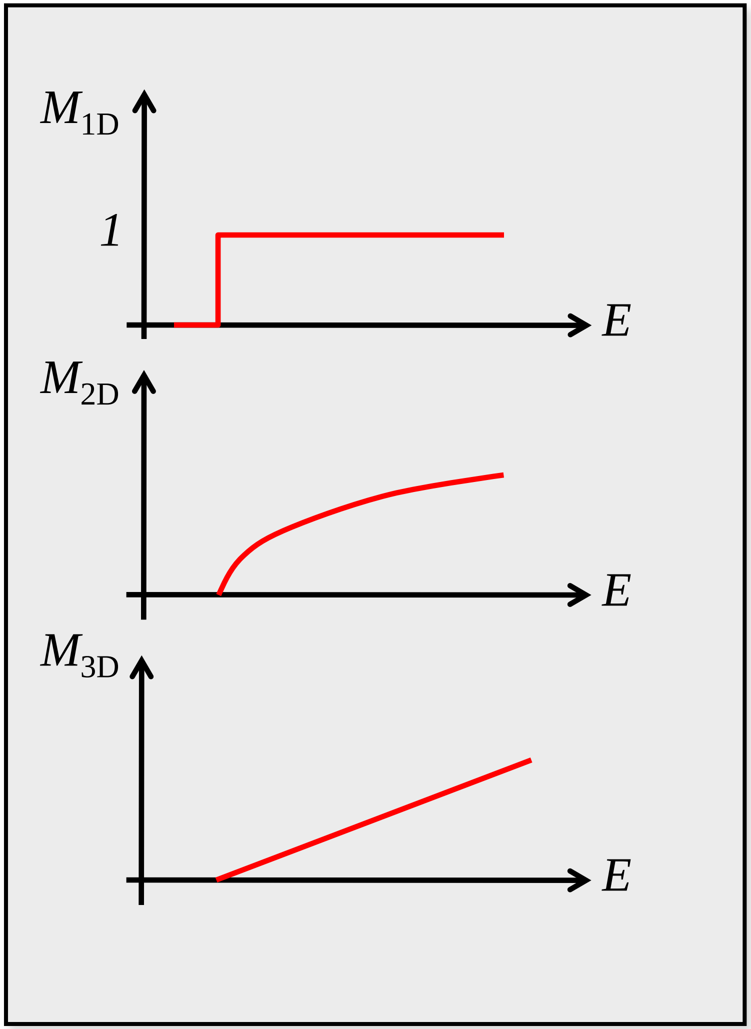
modes

$$M_{1D}\left(E\right) = \Theta\left(E - \varepsilon_1\right)$$

$$M_{2D}\left(E\right) = W\frac{\sqrt{2m^*\left(E - \varepsilon_1\right)}}{\pi\hbar}$$

$$M_{3D}\left(E\right) = A\frac{m^*}{2\pi\hbar^2}\left(E - E_C\right)$$

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



summary

1) When computing the number of electrons, the important quantity is the **density of states, *D*(*E*)**.

2) When computing the current, the important quantity is the **number of modes *M*(*E*)**.

3) The **number of modes** is also the number of subbands at energy, *E*.

4) The **number of modes** is the number of half wavelengths that fit into the resistor width (2D) or cross section (3D).

5) The **number of modes** is proportional to D(E) times velocity.