ECE-656: Fall 2011

Lecture 3: Density of States

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k-space vs. energy-space

$$N_{3D}(k)\,d^3k = \frac{\Omega}{4\pi^3}\,d^3k = D_{3D}\left(E\right)dE$$

N(*k*): independent of bandstructure

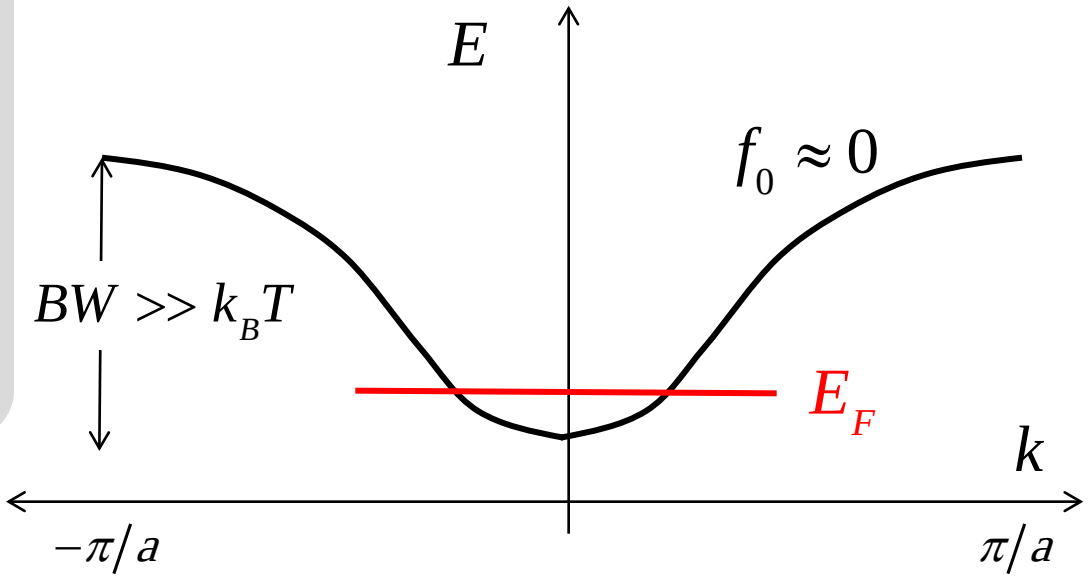
D(E): depends on *E*(*k*)

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 $D_{3D}(E)$ to mean the DOS per unit energy-volume.

about the limits of the integrals

$$n = \frac{1}{4\pi^3}\int_{BZ} f_0\left(E_k\right) d^3k$$

$$n = \frac{1}{4\pi^3}\int_0^{\infty} \frac{4\pi k^2 dk}{1+e^{(E-E_F)/k_BT}}$$



$$f_0 = \frac{1}{1+e^{(E-E_F)/k_BT}}$$

outline

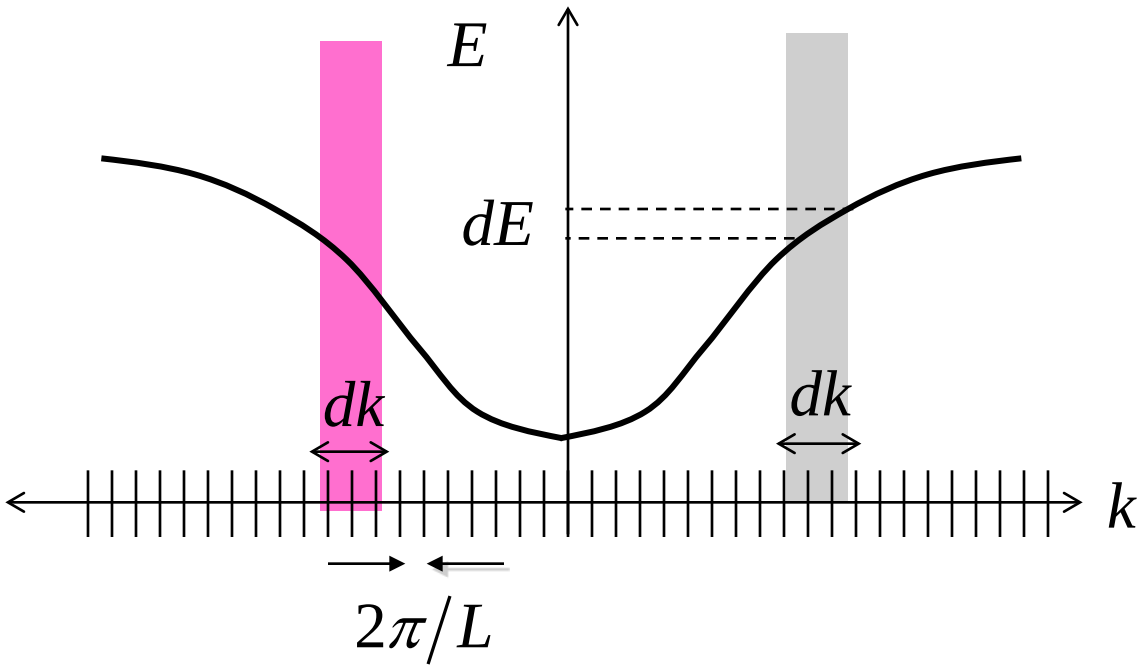
1) **Density of states**

2) Example: graphene

3) Discussion

4) Summary

example: 1D DOS



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

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

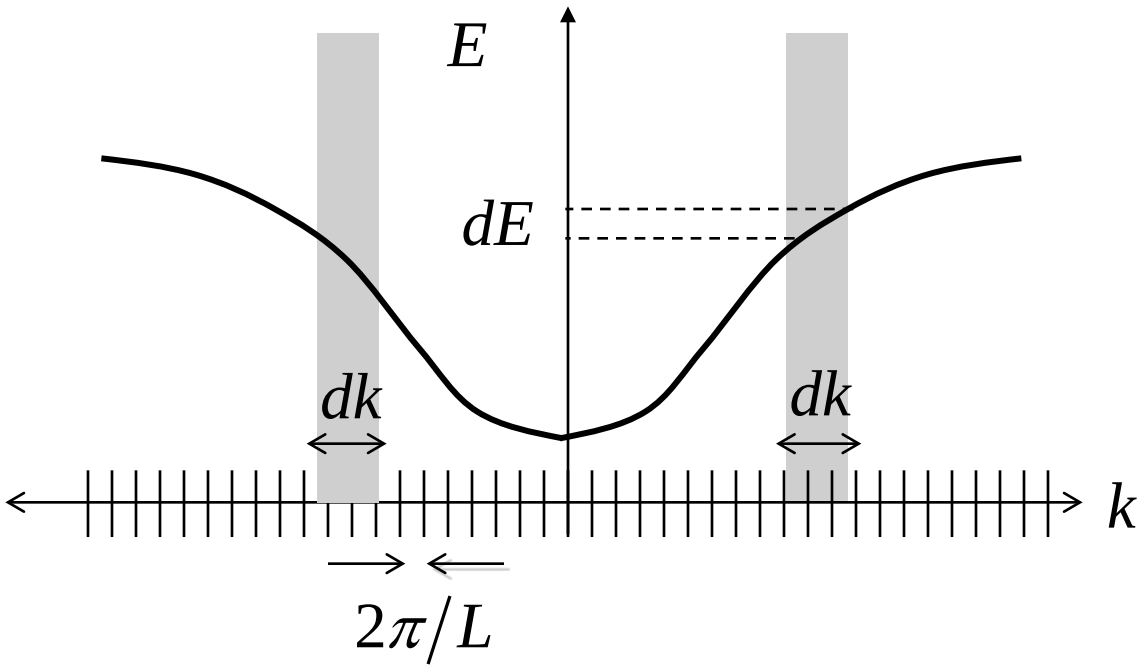
$$D^{+}_{1D}(E)dE = \frac{1}{\pi}dk$$

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

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

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

example: 1D DOS for parabolic bands



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

independent of $E(k)$

parabolic $E(k)$

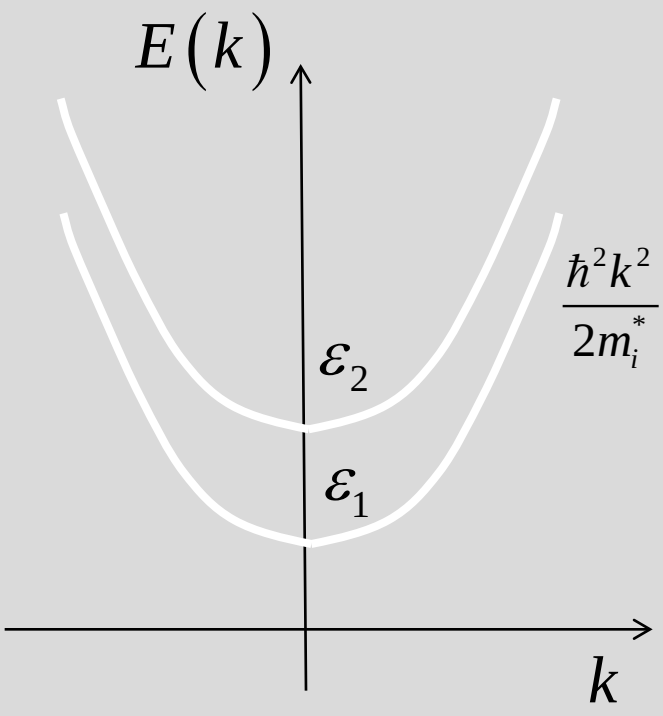
$$E = E_C + \frac{\hbar^2 k^2}{2m^*}$$

$$\upsilon = \frac{1}{\hbar}\frac{dE}{dk} = \sqrt{\frac{2\left(E - E_C\right)}{m^*}}$$

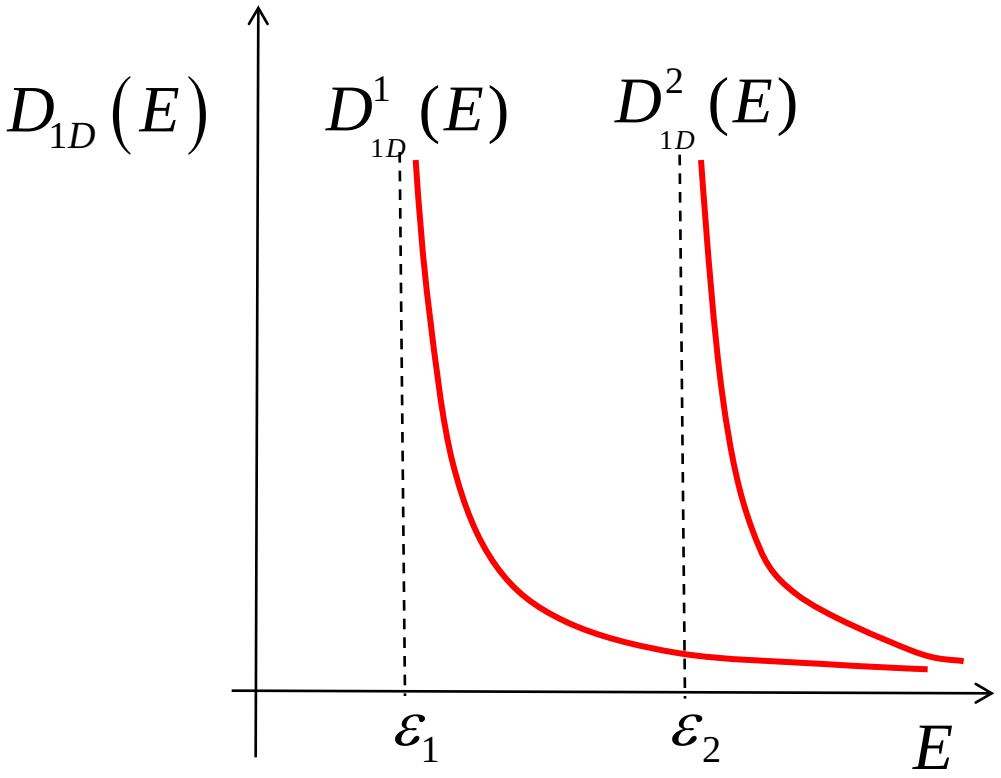
$$D_{1D}(E) = \frac{1}{\pi\hbar}\sqrt{\frac{2m^*}{E - E_C}}$$

density of states in a nanowire

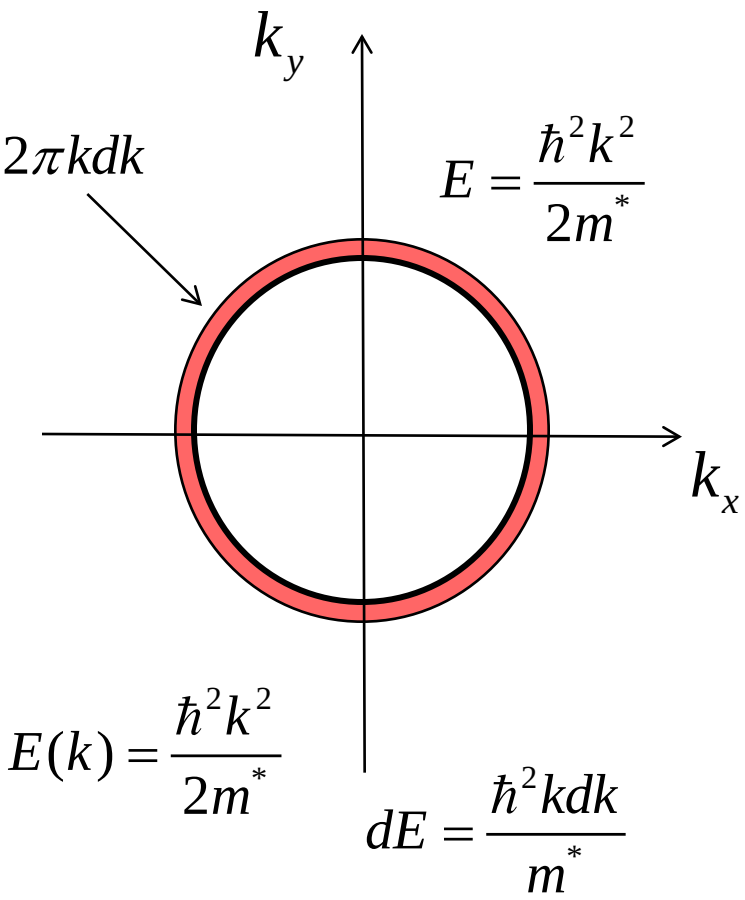
$$E = \varepsilon_i + \frac{\hbar^2 k^2}{2m_i^*}$$



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



2D density of states



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

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

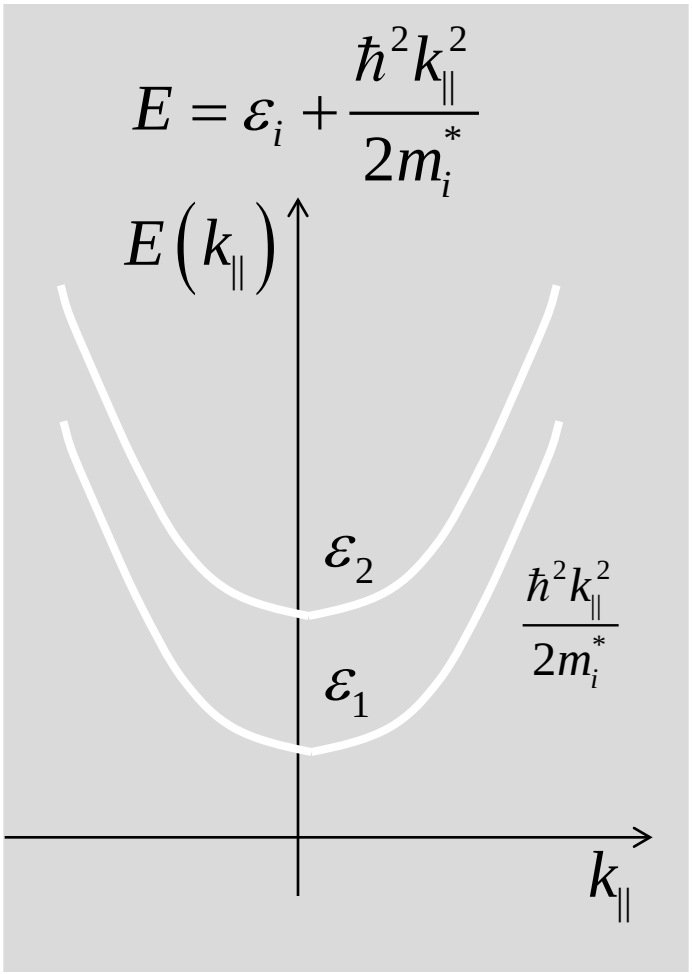
$$D_{2D}(E)dE = \frac{1}{2\pi^2} 2\pi kdk$$

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

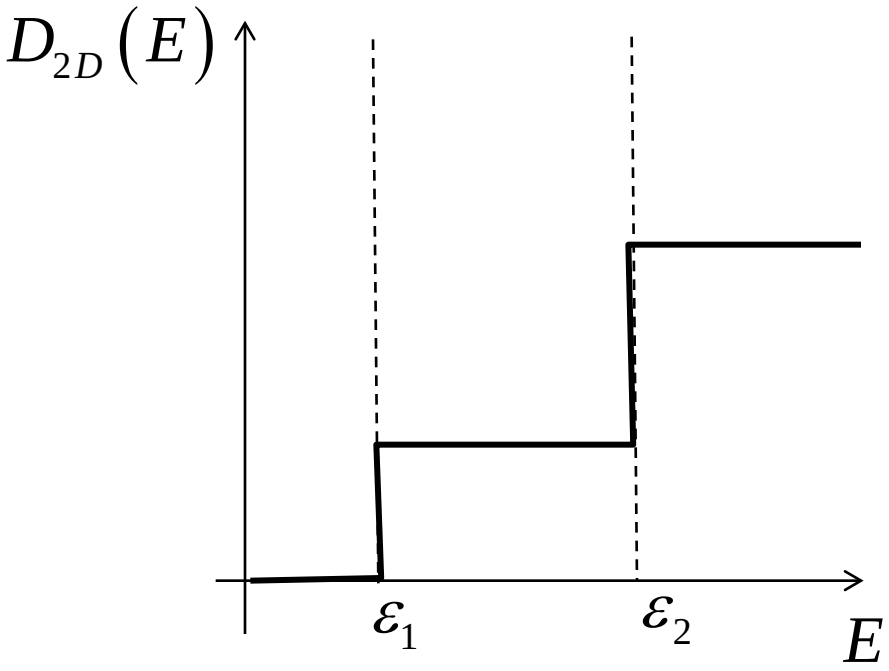
$$D_{2D}(E) = \frac{m^*}{\pi\hbar^2}$$

density of states in a film

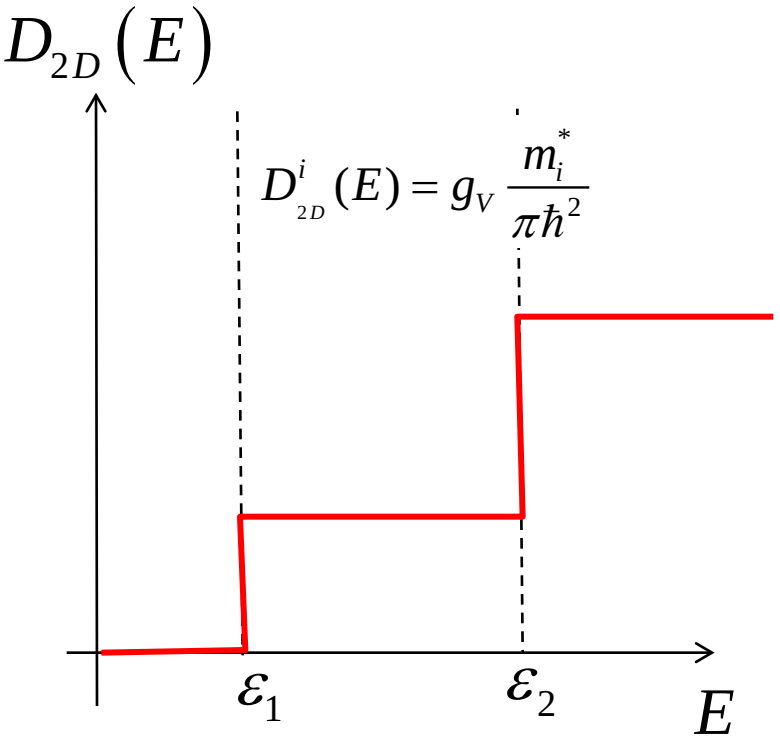
$$E = \varepsilon_i + \frac{\hbar^2 k_{\|}^2}{2m_i^*}$$

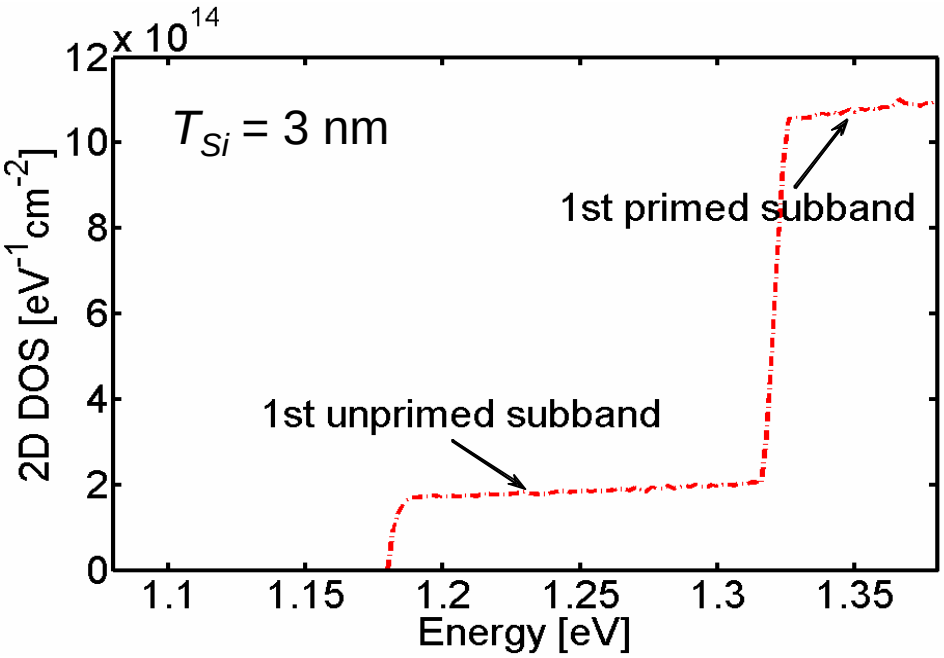


$$D_{2D}^{i}(E) = g_V \frac{m_i^*}{\pi\hbar^2}$$



effective mass vs. tight binding

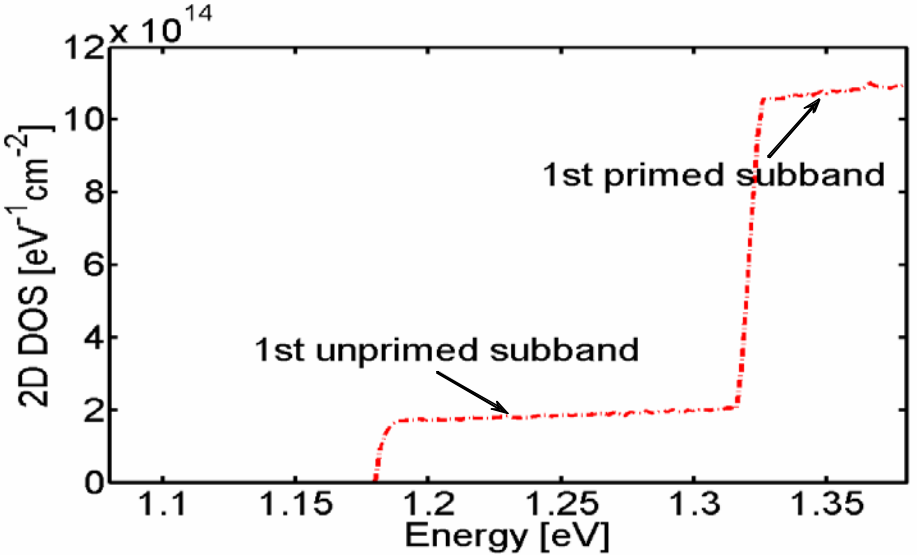




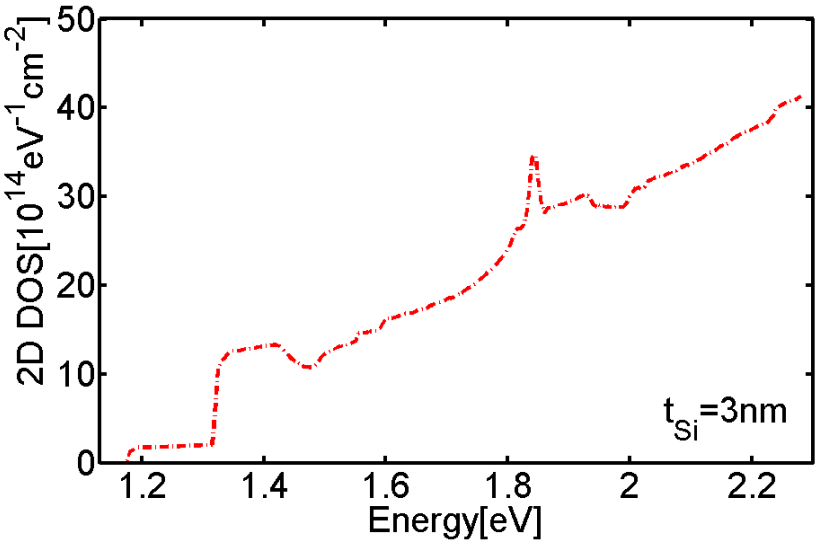
$sp^3s^*d^5$ tight binding calculation by Yang Liu, Purdue University, 2007

effective mass vs. tight binding

near subband edge

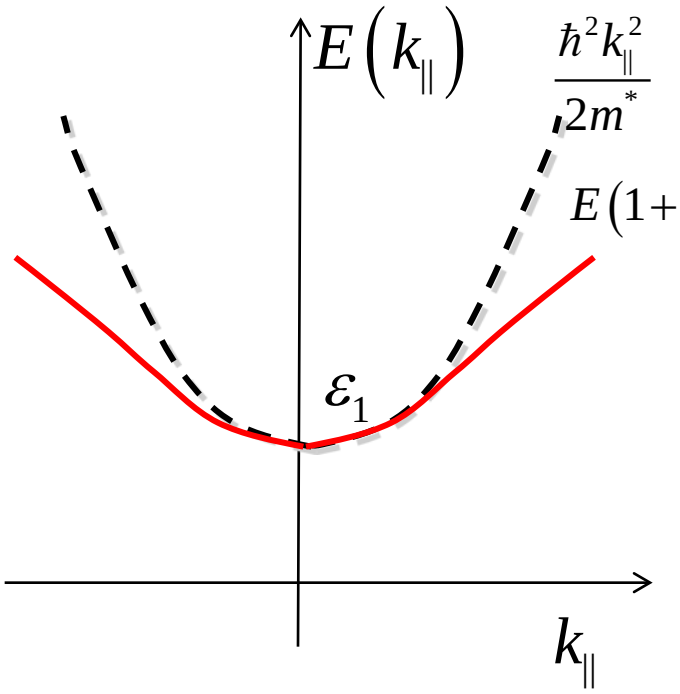


well above subband edge



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

exercise



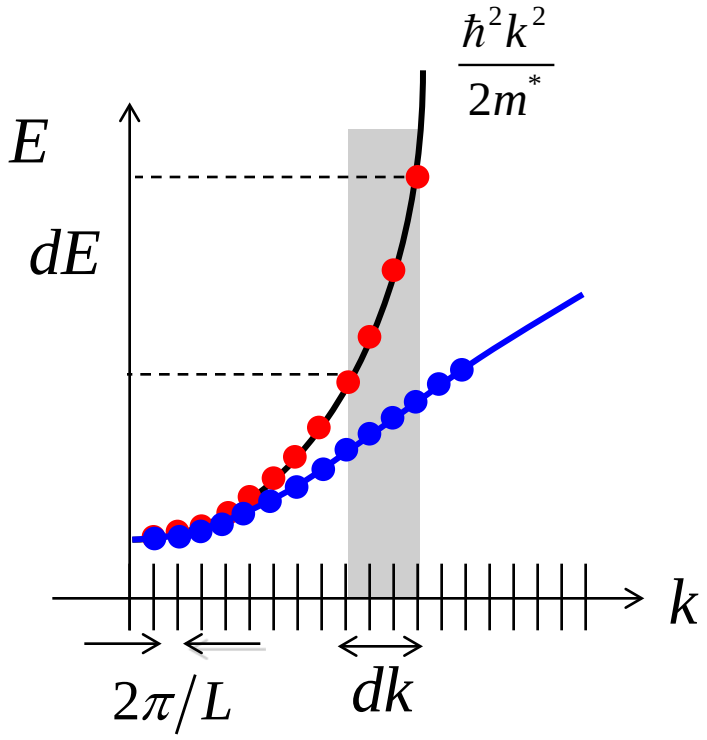
$$E\left(1+\alpha E\right)=\frac{\hbar^2 k_{\|}^2}{2m^*(0)}$$

$$E=\varepsilon_1+E\left(k_{\|}\right)$$

$$E_{k_{\|}}\left(1+\alpha E_{k_{\|}}\right)=\frac{\hbar^2 k_{\|}^2}{2m^*(0)}$$

$$D_{2D}=?$$

how does non-parabolicity affect DOS(E)?



non-parabolicity increases DOS (E)

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:

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

can also work in energy-space:

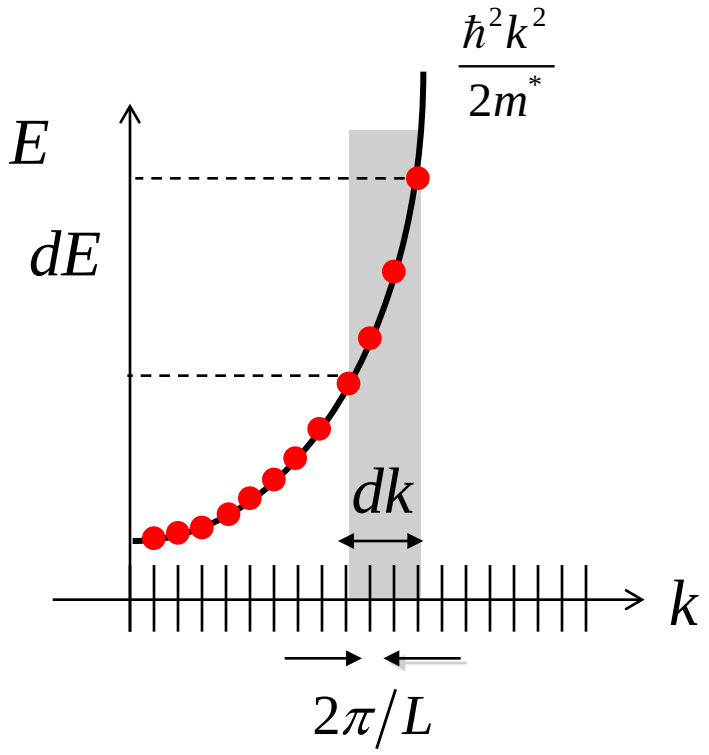
$$n_L = \int f_0\left(E\right) D_{1D}(E)dE$$

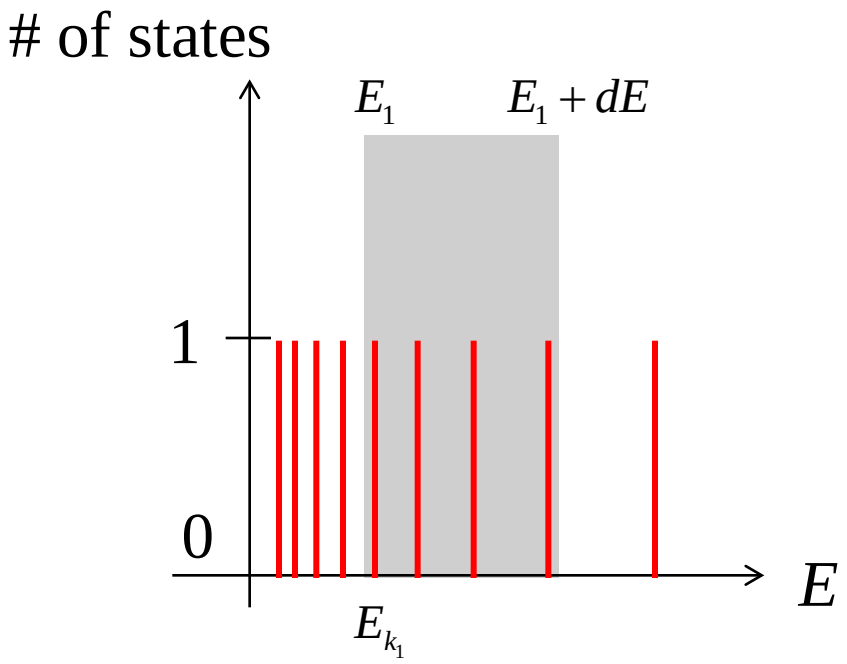
$$n_L = \int f_0\left(E\right)\frac{1}{L}\sum_k \delta\left(E - E_k\right)dE$$

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

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

interpretation





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

counts the states between E and E +dE

outline

1) Density of states

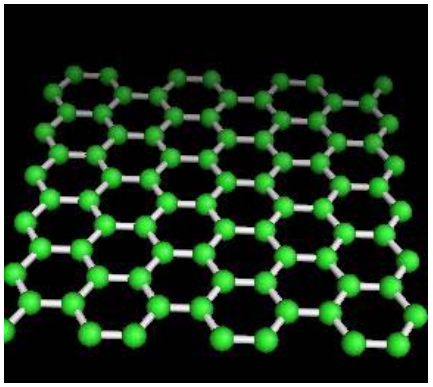
2) **Example: graphene**

3) Discussion

4) Summary

graphene

Graphene is a one-atom-thick planar carbon sheet with a honeycomb lattice.

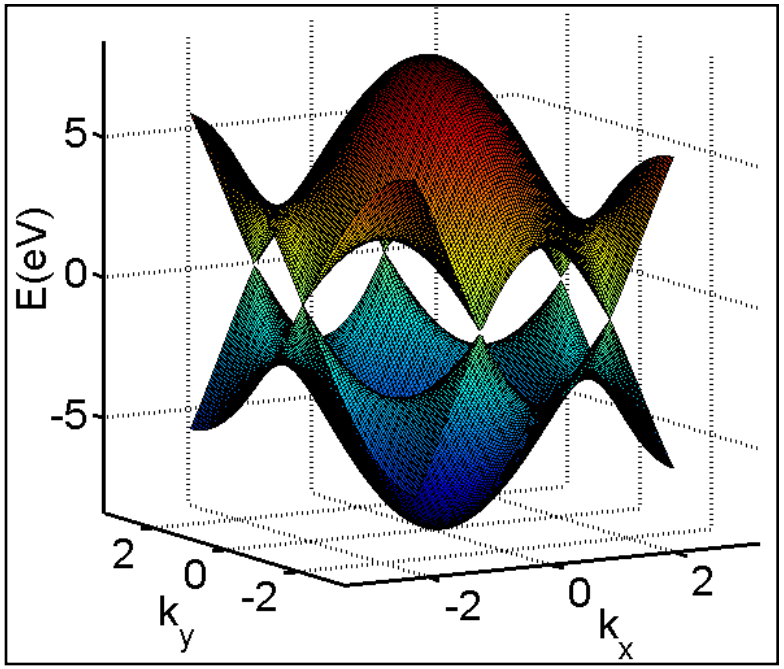


source: CNTBands 2.0 on nanoHUB.org

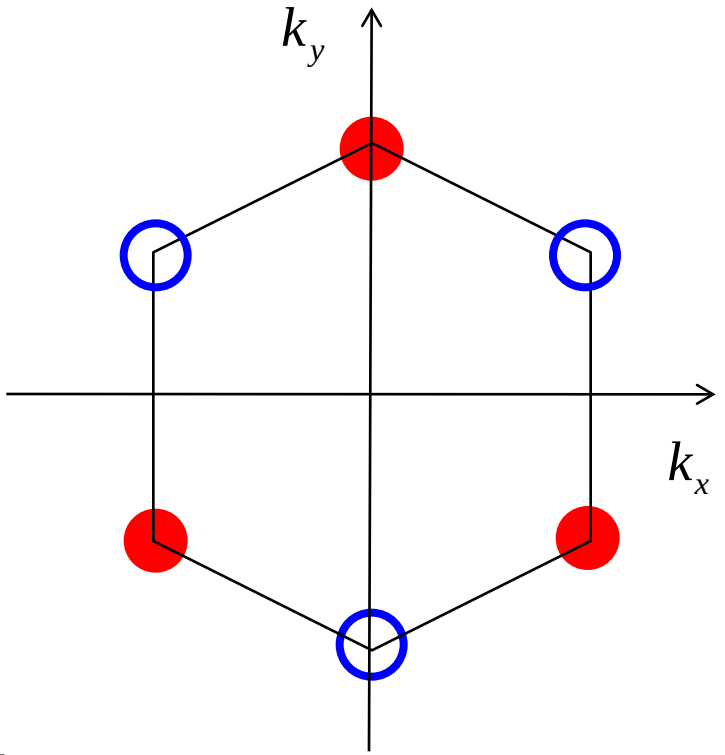
Graphene has an unusual bandstructure that leads to interesting effects and potentially to useful electronic devices.

graphene

E(*k*)



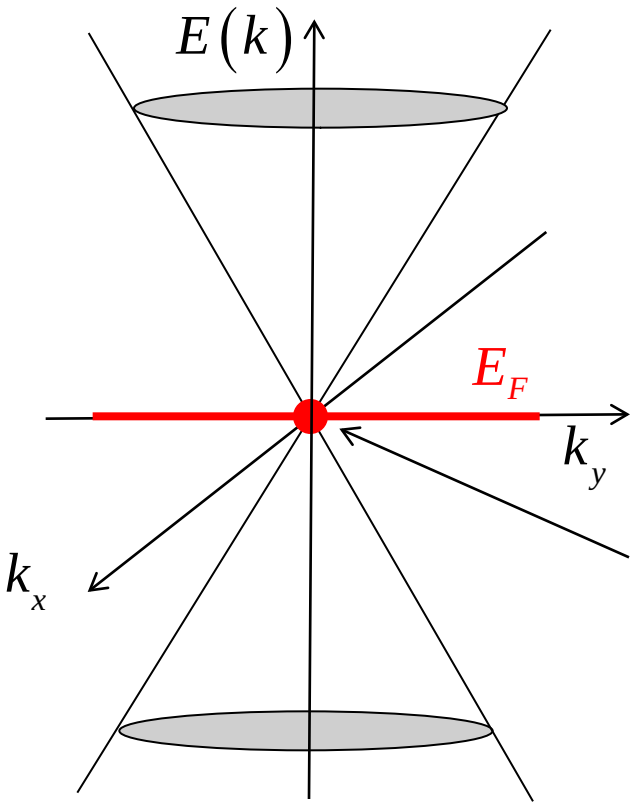
Brillouin zone



Datta: ECE 495N – fall 2008:
https://nanohub.org/resources/5710 (Lecture 21)
https://nanohub.org/resources/5721 (Lecture 22)

simplified bandstructure near $E = 0$

We will use a very simple description of the graphene bandstructure, which is a good approximation near the Fermi level.



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

$$\upsilon(k) = \frac{1}{\hbar}\frac{\partial E}{\partial k} = \upsilon_F$$

$$\upsilon(k) = \upsilon_F \approx 1\times 10^8 \text{cm/s}$$

$g_V = 2$ (valley degeneracy)

"neutral point" ("Dirac point")

We will refer to the $E_F > 0$ case, as "n-type graphene" and to the $E_F < 0$ case as "p-type graphene."

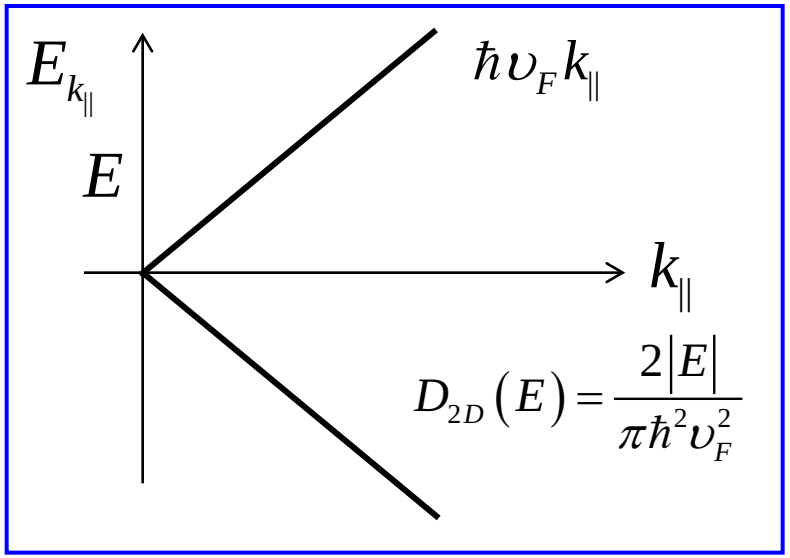
DOS for graphene: method 2

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

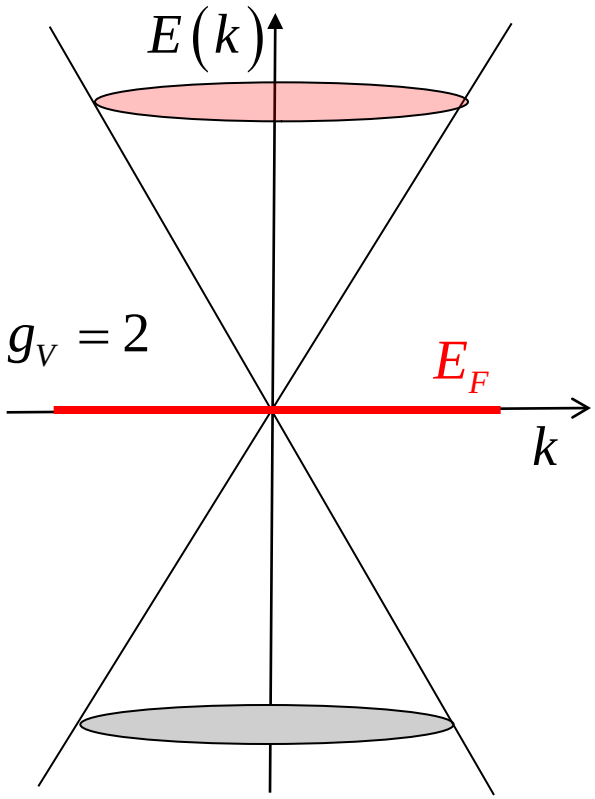
$$E_{k_\parallel} = \hbar\upsilon_F k_\parallel \qquad dE_{k_\parallel} = \hbar\upsilon_F dk_\parallel \qquad k_\parallel\, dk_\parallel = E_{k_\parallel} dE_{k_\parallel} \Big/ \hbar^2\upsilon_F^2$$

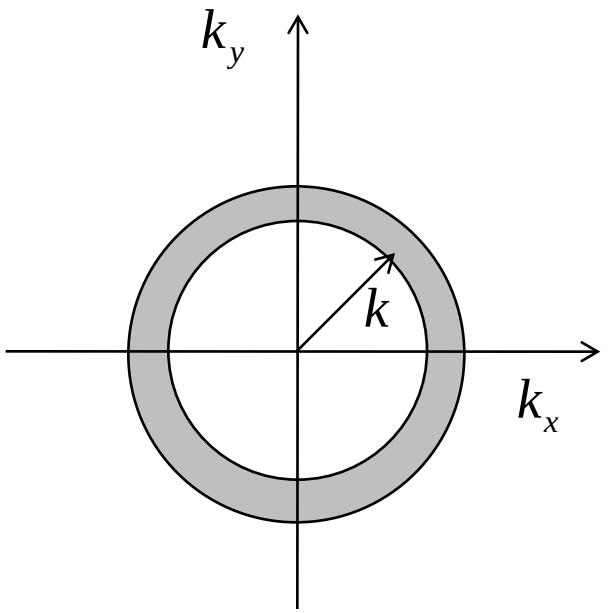
$$D_{2D}(E) = \frac{g_V}{\pi\hbar^2\upsilon_F^2}\int_0^\infty \delta(E - E_{k_\parallel})\,E_{k_\parallel}\, dE_{k_\parallel}$$

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



DOS for graphene: method 1



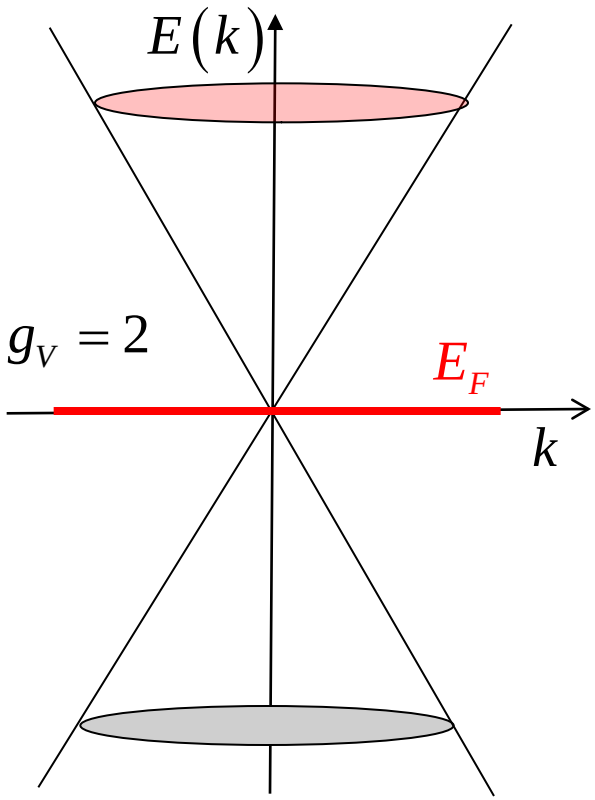


$$N(k)dk = \frac{2\pi\, k dk}{(2\pi/L_x)(2\pi/L_y)} \times 2 \times g_V$$

$$N(k)dk = Ag_V \frac{k dk}{\pi}$$

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

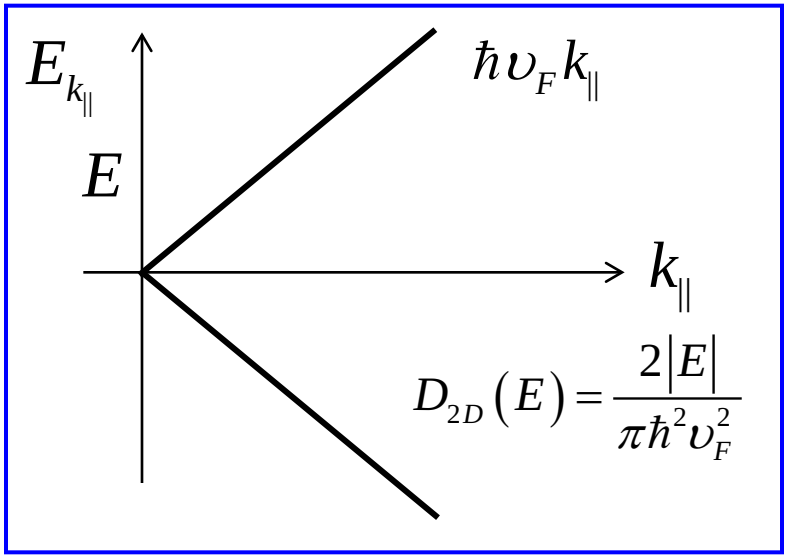
DOS for graphene: method 1



$$N(k)\,dk = Ag_V \frac{k\,dk}{\pi}$$

$$= Ag_V \frac{E\,dE}{\pi(\hbar\upsilon_F)^2}$$

$$= AD_{2D}(E)\,dE$$



outline

1) Density of states

2) Example: graphene

3) **Discussion**

4) Summary

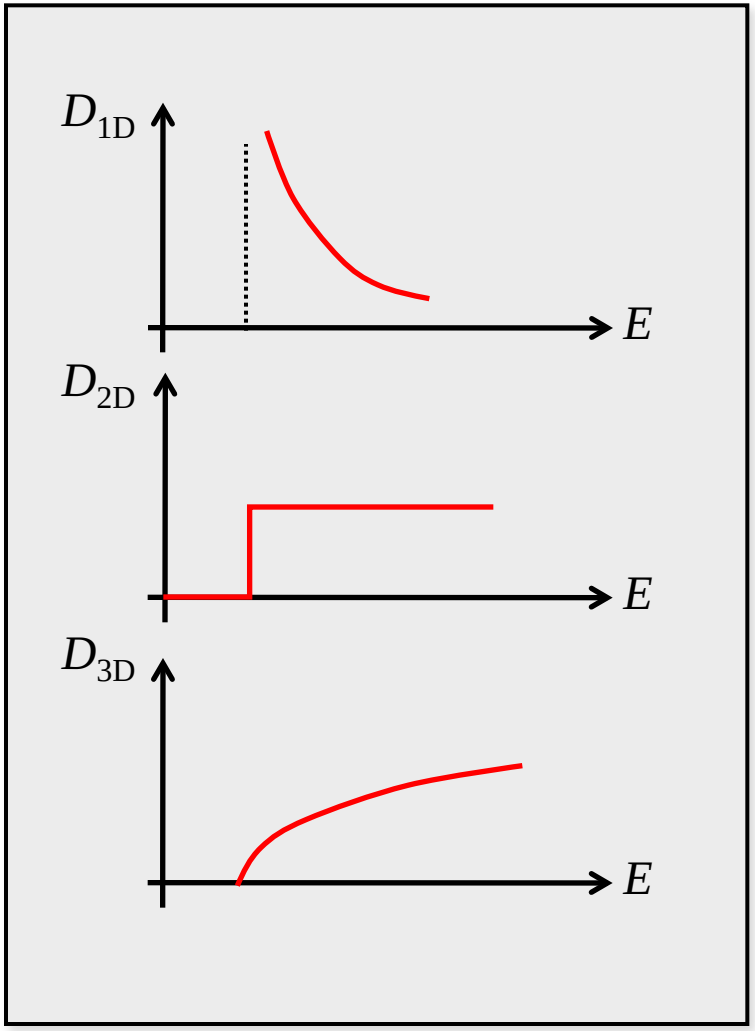
density of states

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

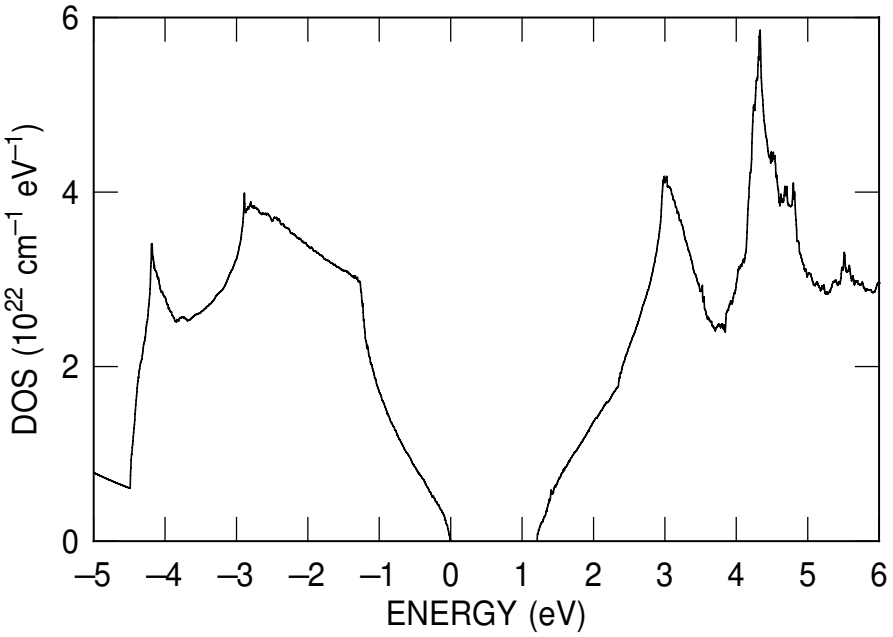
$$D_{2D}(E) = A\frac{m^*}{\pi\hbar^2}\Theta(E-\varepsilon_1)$$

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

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

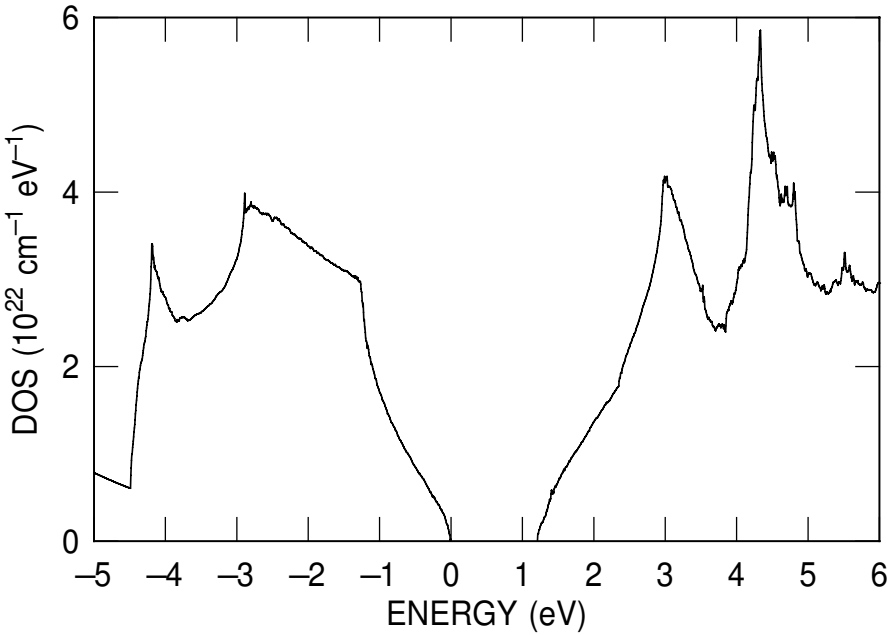


density of states for bulk silicon



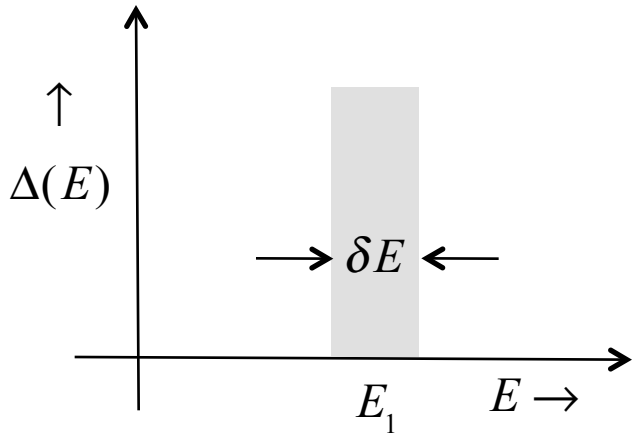
The DOS is calculated with nonlocal empirical pseudopotentials including the spin-orbit interaction.
(Courtesy Massimo Fischetti, August, 2011.)

computing the density of states



Courtesy Massimo Fischetti, August, 2011.

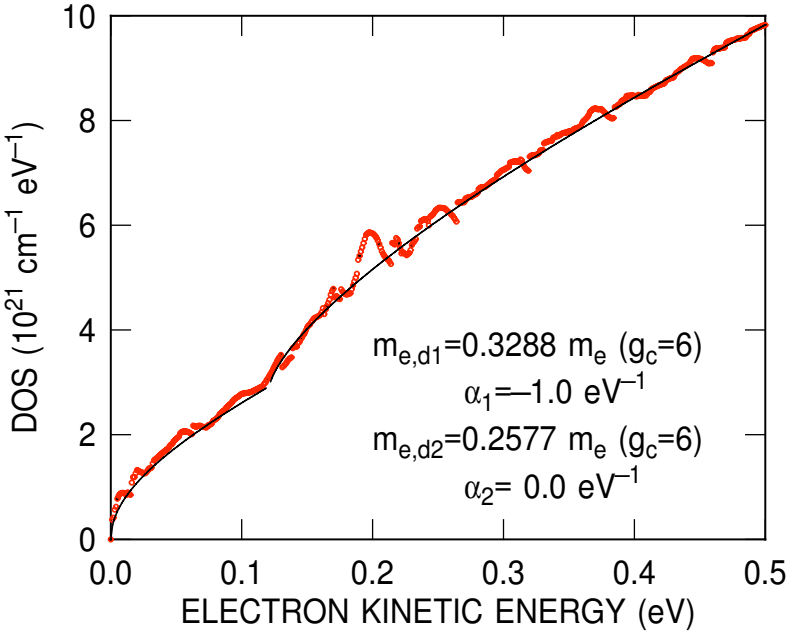
$$D_{3D}(E_1) = \frac{1}{\Omega}\sum_{\mathbf{k}} \delta\left(E_1 - E_{\mathbf{k}}\right)$$



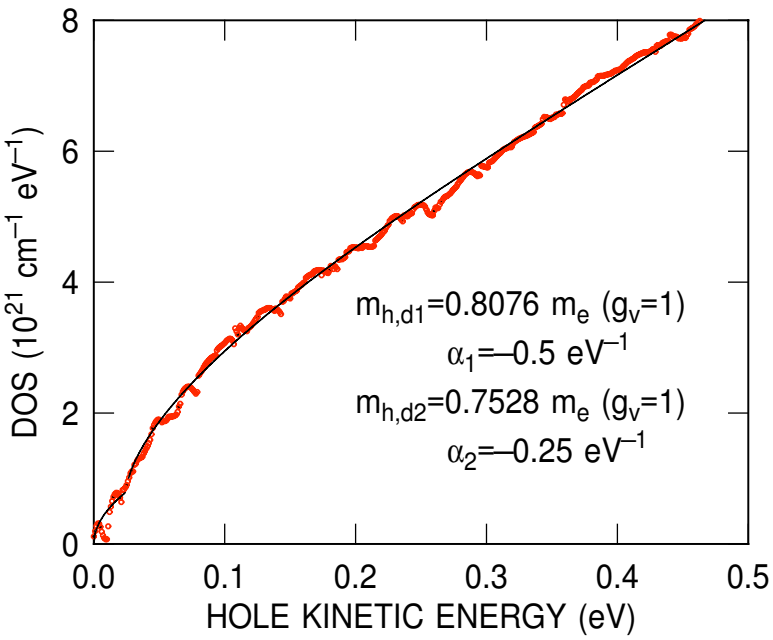
$$\text{no. of states} = \frac{\left(\Delta k\right)^3}{\left(2\pi\right)^3 / \Omega} \times 2$$

density of states for bulk silicon (near the band edge)

conduction band



valence band



(Courtesy Massimo Fischetti, August, 2011)

outline

1) Density of states

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summary

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

2) The DOS depends on dimension (1D, 2D, 3D) and bandstructure.

3) If E(k) can be described analytically, then we can obtain analytical expressions for DOS(E). If not, we can compute it numerically.

questions

1) Density of states

2) Example: graphene

3) Discussion

4) Summary