Fundamentals of Nanoelectronics

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Lecture 24: Density of States (DOS)

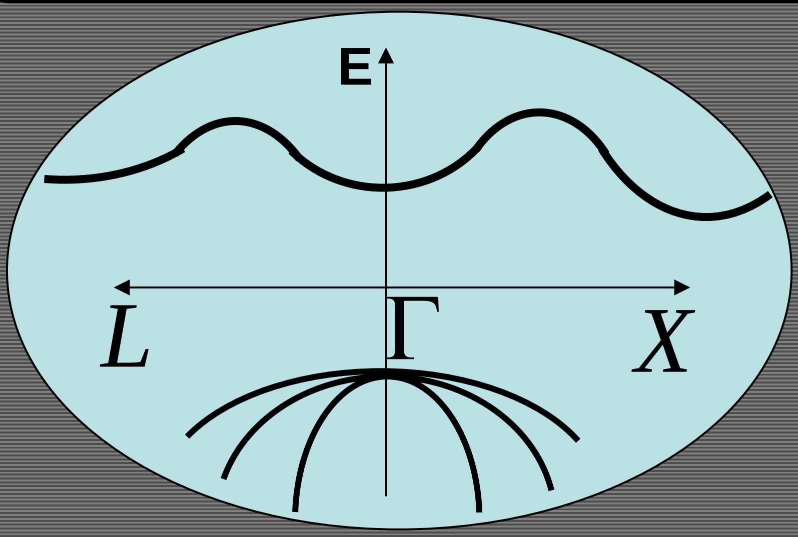
Ref. Chapter 6.2

Network for Computational Nanotechnology

NCN nanoHUB online simulations and more

Overview

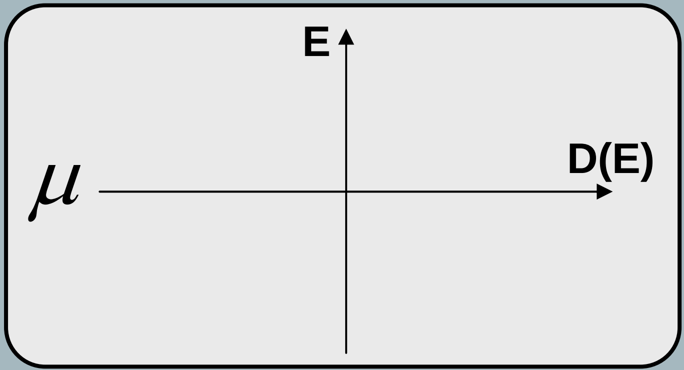
- In the previous lectures we've been talking about E-k diagrams and subbands. What is often measured in experiments is something else called Density Of States (DOS). Therefore what we'll learn next is how to derive DOS from a given E-k relationship.
- In this course we started studying the energy levels of small atoms, then bigger atoms. We continued by studying molecules. Then we studied solids. For solids we classified the energy levels using E-k relationships: E(kx,ky,kz). Take Silicon for example:



- What matter most are the energy levels around the Fermi level because it is those levels that determines the electronic and optical properties.
- In 1970's and 1980's people learned how to make small structures from solids. First the learned confinement in 1D: the resulting material was called a quantum well. Then came confinement in 2D: the resulting material was called a quantum wire. If one confines the solid in all 3 dimension, then we get a quantum dot.
- For quantum wells, wires and dots a good starting point is the E-k relation: E(kx,ky,kz). From there one can confine each dimension one by one:
- $$E_v(k_x,k_y) = E\left(k_x,k_y,k_z=\frac{v\pi}{L_z}\right)$$
- $$E_{v,v'}(k_x) = E\left(k_x,k_y=\frac{v'\pi}{L_y},k_z=\frac{v\pi}{L_z}\right)$$
- $$E_{v,v',v''} = E\left(k_x=\frac{v''\pi}{L_x},k_y=\frac{v'\pi}{L_y},k_z=\frac{v\pi}{L_z}\right)$$

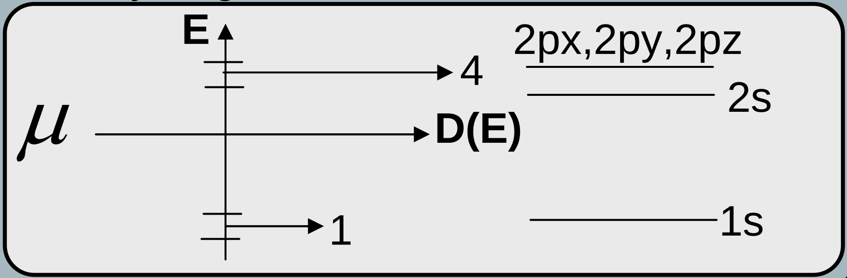
Overview: From E-k to DOS

• What we want to talk about today is turning a given E-k diagram and turning it into a DOS plot:

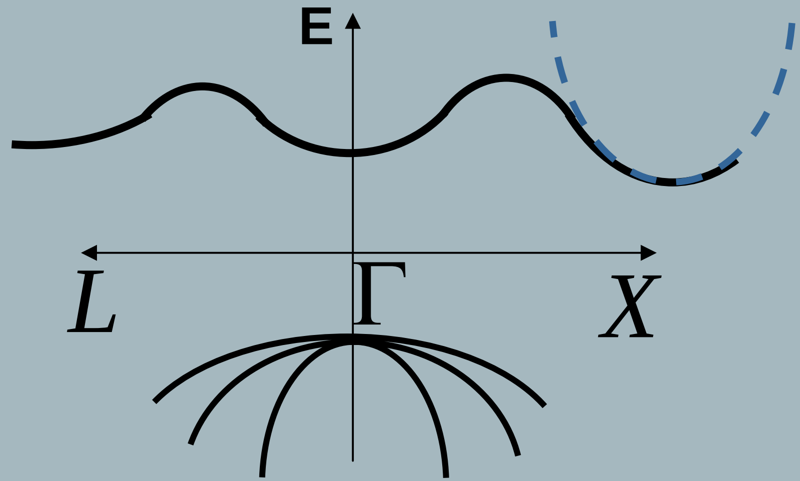


• What this plot will tell is the density of states in a given energy range. For example having D(E)=10/eV results in 10 energy levels in a 1eV range of energy.

• For Hydrogen atom we'll have:



• Next consider Silicon:



• Since we are interested in the energy levels around the Fermi level, for conduction band, the minimum is important and no matter how complicated the E-k relation, we can approximate it as a parabola for a small energy range. Naively speaking for the parabola in the case of Si we have:

$$E = E_C + \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

E-k to DOS: 1D

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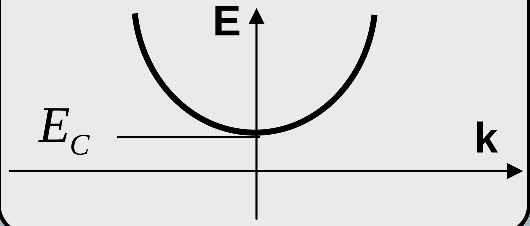
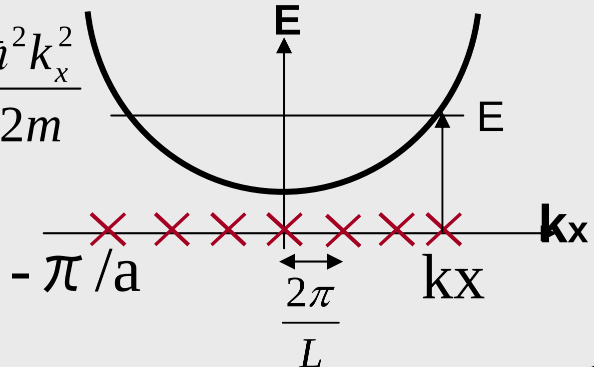


$$E = E_C + \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2 + k_z^2\right)$$

- How can we get from here to DOS?
- To make it simpler consider a 1D solid:

(1)
$$E = E_C + \frac{\hbar^2 k_x^2}{2m}$$



- First let's try to write the total number of states below E denoted as: $N_T(E)$

- Consider a 1D solid with length L. The allowed values of kx will be (using 1):

$$k_x = \frac{\sqrt{2m\left(E - E_c\right)}}{\hbar}$$

- In terms of kx we have:

$$N_T(k_x) = \frac{k_x}{2\pi / L}$$

- D(E) is actually the derivative of the total number of states:

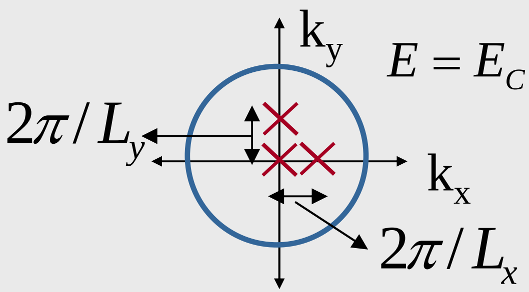
$$D(E) = \frac{L}{\pi}\left(\frac{dk_x}{dE}\right) = \frac{L/\pi}{dE/dk_x}$$

$$= \frac{L/\pi}{dE/dk_x} = \frac{L/\pi}{\hbar k_x / m}$$

$$= \frac{L}{\pi}\frac{m}{\hbar\sqrt{2m\left(E - E_c\right)}}$$

E-k to DOS: 2D

- For 2D we have:



$$E = E_C + \frac{\hbar^2}{2m}\left(k_x^2 + k_y^2\right)$$

- The question to be asked is that how many states we have inside the circle above? In 1D we looked at the total length. In this case we look at the area of the circle considering the fact that each state occupies the area of:

$$\left(2\pi/L_x\right)\left(2\pi/L_y\right)$$

- We need to know how many of above can be fit into the circle. That will be the total number of states:

$$N_T(k) = \frac{\pi\left(k_x^2 + k_y^2\right)}{\frac{2\pi}{L_x}\frac{2\pi}{L_y}}$$

- If we substitute: Lx Ly=S, then

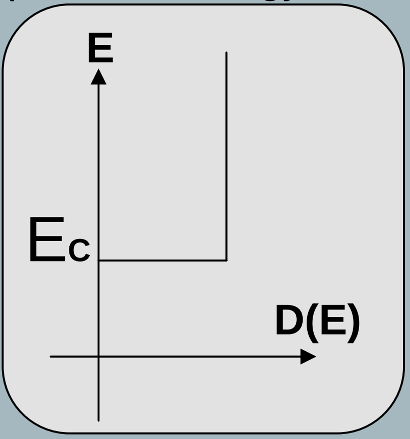
$$N_T(k) = \pi k^2 \, S \big/ 4\pi^2 \qquad k^2 = k_x^2 + k_y^2$$

- For D(E) we have:

$$D(E) = \frac{S}{4\pi^2}\pi\frac{d}{dE}\left(k^2\right) = \frac{S}{4\pi^2}\pi\frac{2m}{\hbar^2}$$

$$\boxed{D(E) = \frac{Sm}{2\pi\hbar^2}}$$

- One point to notice is that in this case, DOS does not depend on energy.



E-k to DOS: 3D

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- For 3D, again we need to write down the total number of states below a certain energy level.

$$N_T(k) = \frac{\frac{4}{3}\pi k^3}{\frac{2\pi}{L_x}\frac{2\pi}{L_y}\frac{2\pi}{L_z}} = \frac{\Omega}{8\pi^3}\frac{4\pi}{3}k^3$$

$$\Omega = L_x L_y L_z$$

$$k = \sqrt{k_x^2 + k_y^2 + k_z^2}$$

$$D(E) = \frac{\Omega}{8\pi^3}\frac{4\pi}{3}\left(\frac{dk^3}{dE}\right) = \frac{\Omega}{8\pi^3}\frac{4\pi}{3}3k^2\frac{dk}{dE} = \frac{\Omega}{8\pi^3}\frac{4\pi}{3}\frac{3k^2}{dE/dk} \Rightarrow$$

$$\boxed{D(E) = \frac{\Omega}{2\pi^2\hbar^3}\left[2m\left(E - E_c\right)\right]^{1/2}}$$

E-k to DOS: Graphene

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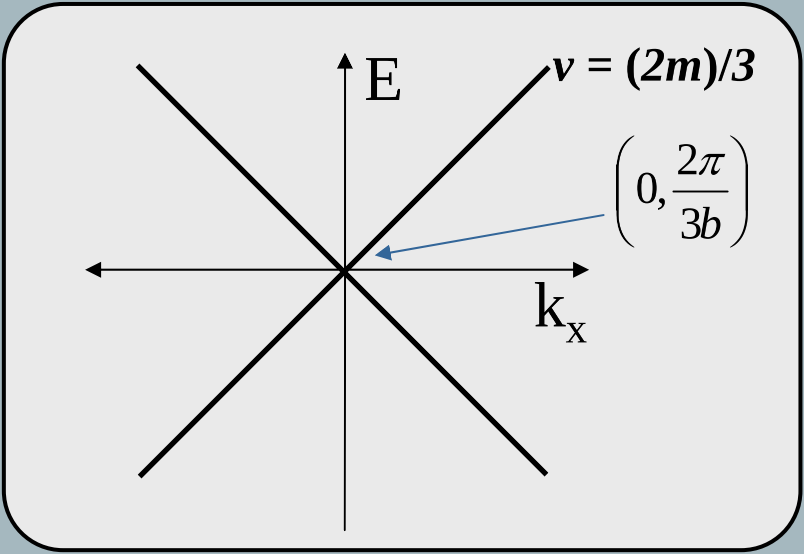
- The energy eigenvalues for Graphene were approximated as:

$$E_v(k_x) = \varepsilon + \frac{3a_0 t}{2}\sqrt{k_x^{\,2} + k_y^{\,2}}$$

- Consider the E-k diagram:



- We are interested in how many states lie within a region of radius k, such that

$$N(k) = \pi k^2 \, S \big/ 4\pi^2$$

where s is the surface area of a 2-D material such as graphite

- By nature, of course, we wish to express N in terms of energy. For graphite we use

$$D(E) = \frac{\partial N(E)}{\partial E} = \frac{S}{4\pi}\frac{2k}{dE/dk}$$

$$D(E) = \frac{S}{4\pi}\frac{2(E-\varepsilon)}{3ta_0/2}$$