Fundamentals of Nanoelectronics

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Lecture 25: Density Of States: General Approach

Ref. Chapter 6.2

Network for Computational Nanotechnology

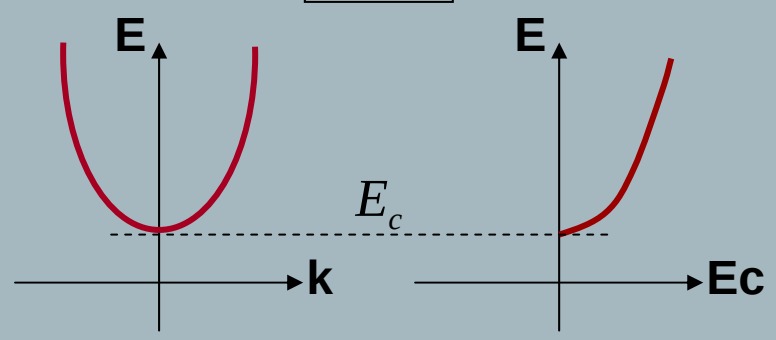
NCN
nanoHUB
online simulations and more

Preview/Review

00:03

- We like to be able to learn DOS in a more general sense. The dispersion relation can be used to derive DOS with this fact in mind that the dispersion relation exists only for periodic structures. Note that even without dispersion relation, DOS still exists. In that sense DOS is a more fundamental concept than dispersion relation.
- Remember what we've done last day:

3-D

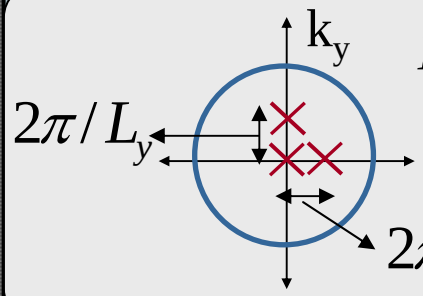


$$E = E_c + \frac{\hbar^2 k^2}{2m} \Rightarrow D(E) \propto \sqrt{\mathrm{E - E_c}}$$

From E-k to DOS
N(k) → N(E) → D(E)

02:30

- For 2D we have:



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

Periodic boundary conditions are assumed

- 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

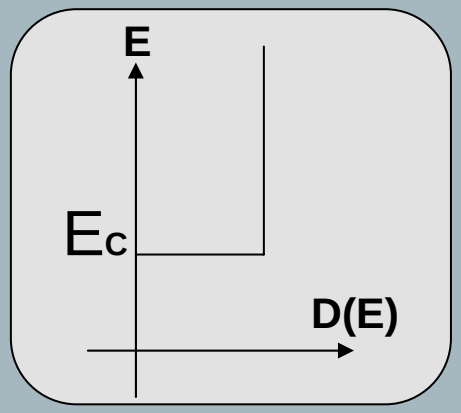
$$N_T(k) = \pi k^2 \, S/4\pi^2 \qquad k^2 = k_x^2 + k_y^2$$

- 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.



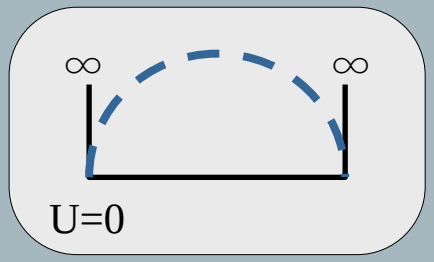
Periodic BC versus Infinite Wall BC

05:02

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

• Notice that the 2pi/Lx in the above relation is the result of Periodic Boundary Conditions (PBC). This may not be necessarily true for solids but the physical argument is that what happens at the boundaries does not affect the center and we are interested in the center. Assuming PBC means: $k_x L_x = 2\pi\nu_x$

• Another approach would be to assume infinite potential wall Boundary Conditions (BC).



• In this case wavefunctions have to go to zero at the two ends. If so instead of exponentials, “sin” functions are the from of solutions.

$$\sin k_x x \Rightarrow k_x L_x = \pi\upsilon \Rightarrow \; k_x = \left(\pi/L_x\right)\upsilon$$

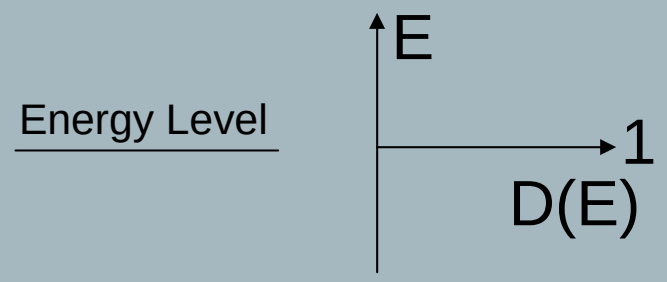
• This means that k states will be pi/Lx apart instead of 2pi/Lx of periodic boundary conditions. Does this mean that we have twice as many states?

• The answer is no. For PBC solutions are exponential and exp(ikx) is linearly **in**dependent of exp(–ikx). So there are actually two solutions for k and – k. How ever in the case of “sin” function: sin(-kx)= –sin(kx). You can clearly see that these are two linearly **d**ependent answers. In summary again:

N(k) → N(E) → D(E)

Overview: DOS (General Approach)

- Given any piece of solid its energy levels can be described by the eigenvalues of the Hamiltonian matrix [H] for that solid. These eigenvalues can be denoted as ε_α . Alpha is the subscript that indicates which eigenvalue we are considering.
- What would DOS be if we had only one energy level? It would be a delta function.



- So for each energy level we have a delta function of strength 1. So we can write DOS as:

$$D(E) = \sum_\alpha \delta\left(E - \varepsilon_\alpha\right)$$

DOS: General Approach 1D

15:24

- Let's try to do this for 1-D. If we have dispersion relation like: $E = E_c + \frac{\hbar^2 k^2}{2m}$
- Then we can write DOS in terms of k states: $D(E) = \sum_k \delta(E - \varepsilon_k)$

- If the states are really closely spaced then we can write the summation as an integral:

Useful identities for the integration below

$$\boxed{\int \delta(E)dE = 1} \qquad \boxed{\int \delta(E-\varepsilon)dE = 1} \qquad \boxed{\int \delta(\varepsilon - E)d\varepsilon = 1}$$

$$\varepsilon_k = E + \frac{\hbar^2 k^2}{2m} \Rightarrow \boxed{\frac{d\varepsilon_k}{dk}} = \frac{\hbar^2}{m}\frac{\sqrt{2m(\varepsilon_k - E_c)}}{\hbar} = \frac{\hbar\sqrt{2m(\varepsilon_k - E_c)}}{m}$$

$$D(E) = \sum_k \delta(E-\varepsilon_k) = 2\frac{L}{2\pi}\int dk\,\delta(E-\varepsilon_k) = 2\int \frac{d\varepsilon_k . L}{2\pi}\boxed{\frac{dk}{d\varepsilon_k}} = \int \frac{d\varepsilon_k . L}{2\pi}\frac{m}{\hbar\sqrt{2m(\varepsilon_k - E_c)}}\delta(E-\varepsilon_k)$$

$$\boxed{\text{Identity: } \int dE\,\delta(\varepsilon - E)f(\varepsilon) = f(E)}$$

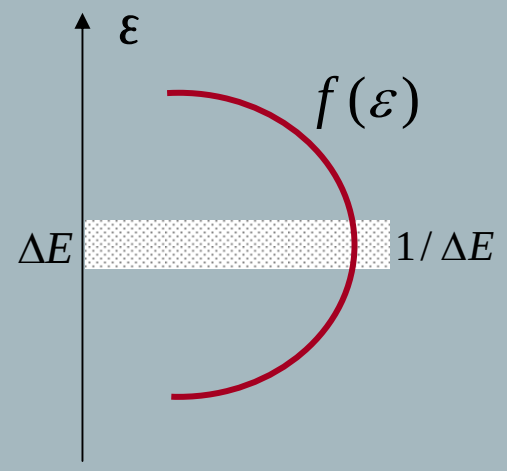
$$\boxed{D(E) = 2\frac{L}{2\pi}\frac{m}{\hbar\sqrt{2m(E-E_c)}}}$$ 1D

A Note About Delta Function

- To derive DOS in 1D we used the following identity:

$$\int dE\delta(\varepsilon - E) f(\varepsilon) = f(E)$$

- Consider the picture below to see why:

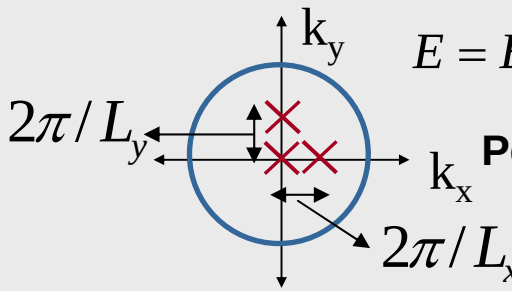


$$\int dE\delta(\varepsilon - E) f(\varepsilon) = f(E)$$

DOS: General Approach 2D

35:30

- Let's derive DOS for a 2D solid:



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

Periodic boundary conditions are assumed

$$D(E) = \sum_{k_x,k_y} \delta\left(E - \varepsilon_{k_x,k_y}\right) = \int \frac{dk_x L_x}{2\pi} \int \frac{dk_y L_y}{2\pi} \delta\left(E - \varepsilon_k\right) = \frac{S}{4\pi^2} \int dk_x dk_y \delta\left(E - \varepsilon_k\right)$$

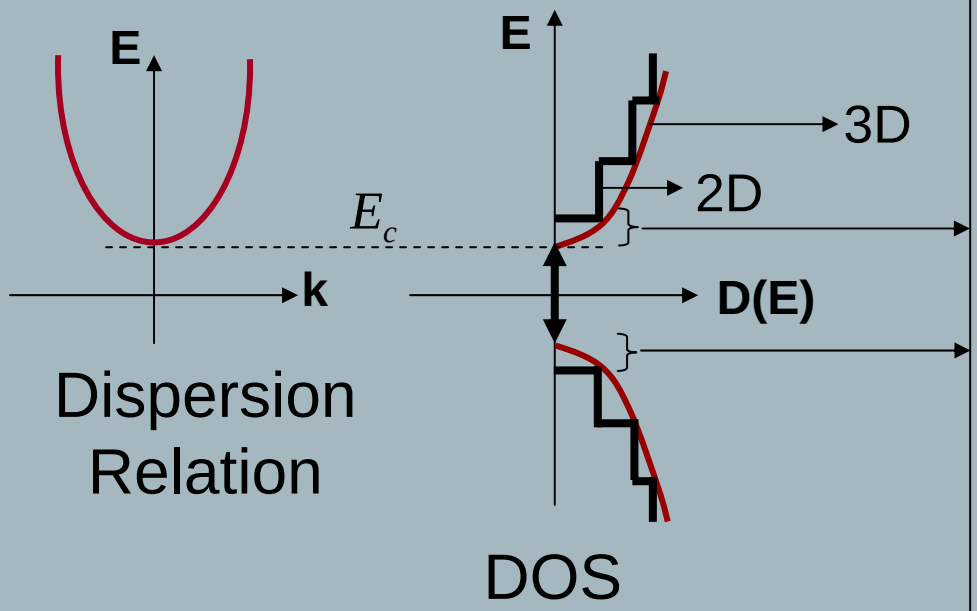
- Putting this is circular coordinates…

$$D(E) = \frac{S}{4\pi^2} \int 2\pi k dk \delta\left(E - \varepsilon_k\right) = \frac{S}{2\pi} \int \frac{k d\varepsilon_k}{d\varepsilon_k / dk} \delta\left(E - \varepsilon_k\right) = \frac{Sm}{2\pi\hbar^2} \int d\varepsilon_k \delta\left(E - \varepsilon_k\right)$$

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

Blue Shift

43:30



This gap is due to confinement. As one goes form 3D to 2D the solid is confined in 1 dimension and the energy levels become discretized in that direction. The ground state energy will not be the bottom of conduction band. This has confirmed to be the case by optical experiments. Whereas the gap between the conduction band edge and valence bad edge is 1.5eV, the photon that is emitted by the material has higher energy indicating that the first energy levels occur higher than the conduction band edge and lower than valence band edge. For 3D the light is in infrared range and for 2D the light shifts towards shorter wavelengths of blue range. Because of this, people call this type of confinement the blue shift.