# Fundamentals of Nanoelectronics

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## Lecture 26: DOS in Nanostructures

Ref. Chapter 6.2

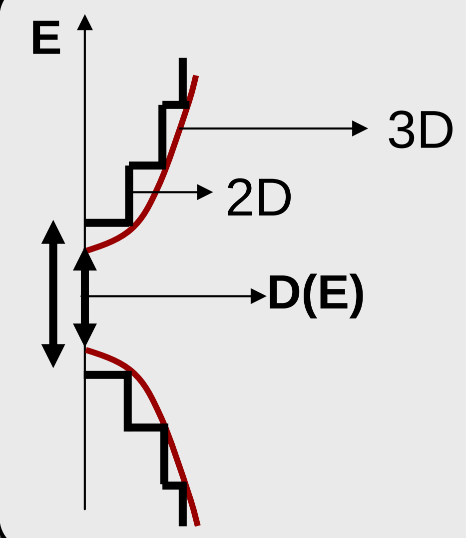
*Network for Computational Nanotechnology*

NCN nanoHUB online simulations and more

# Confinement → Change In DOS



- When one makes a nanostructure out of a large piece of solid, one of the most observable effects is the change in DOS. The figure compares the 3D DOS and a solid confined in 1 direction: 2D.
- One can run current through the device and obtain information about the shape of DOS. Obviously the two characteristics will be different.
- What is even more striking is the difference in the optical properties. You can see from the figure that the 3D DOS has a smaller bandgap than 2D DOS. This results in higher frequency of the emitted light for the 2D solid. The emitted light from the 3D gap is in the infrared region. The higher gap of 2D means higher energy or equivalently higher frequency of emitted light. Since this shift infrequency is towards the blue region, this phenomenon is called the blue shift.

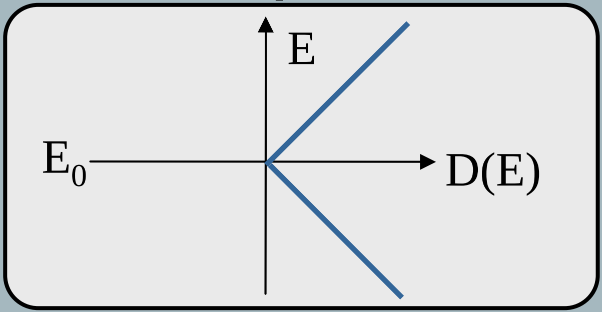


# Overview

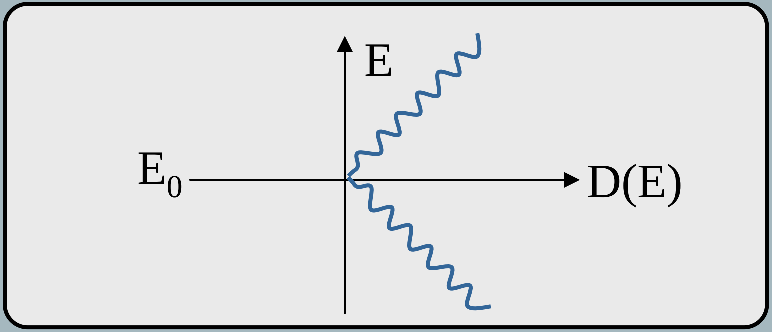


- In the previous lectures we've seen how one can derive DOS from a dispersion relation. Today we'd like to do this for Graphene and a rolled up Graphene, i.e. a Carbon Nanotune.
- Let's see the results first:

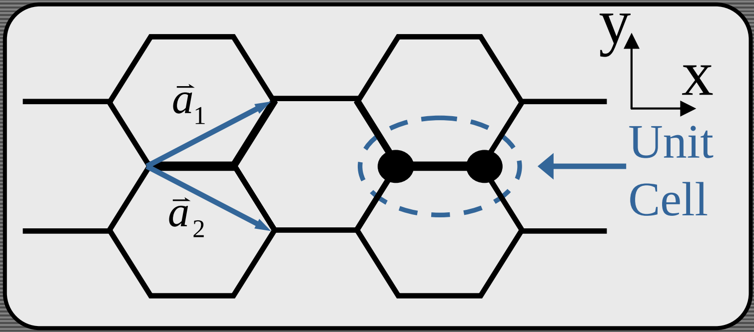
**Graphene**




**Carbon Nanotube**



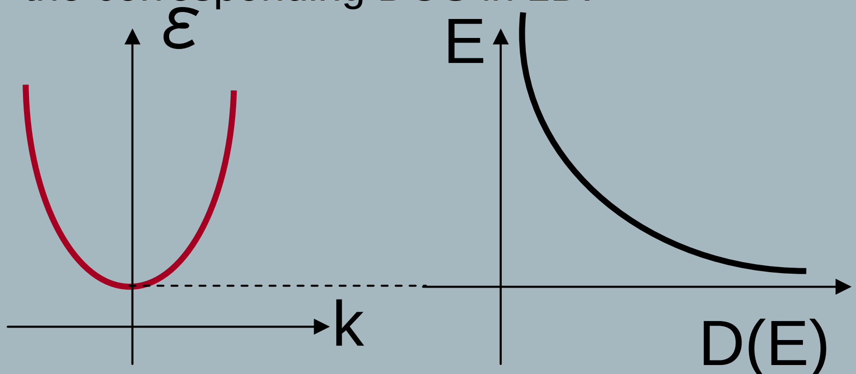

**Graphene**



# DOS For a 1D Nano Wire



• A point about any dispersion relation and the corresponding DOS in 1D.




• DOS is inversely proportional to the slope of the dispersion curve. Where the slope is zero, DOS is very high. That is in 1D

$$\boxed{D(E)=\frac{1}{\pi\, {d\varepsilon}/{dk}}}$$

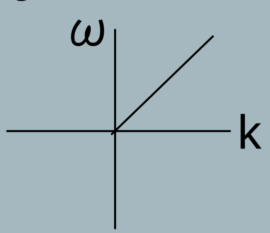
• Reminder:

$$D(E)=\sum_k \delta(E-\varepsilon_k)=2\frac{L}{2\pi}\int dk\,\delta(E-\varepsilon_k)$$

$$=\int \frac{d\varepsilon_k.L}{\pi}\frac{dk}{d\varepsilon_k}=\frac{1}{\pi\, {d\varepsilon}/{dk}}$$

• Notice that the results should include a factor of 2 if one wants to include spin degeneracy.

• Another thing is to notice the group velocity.




$$v=\frac{d\omega}{dk}$$

• So we can rewrite DOS:

1D: $$\boxed{D(E)=\frac{1}{\pi\hbar v}}$$

# Dispersion Relation
# Graphene → Nanotube

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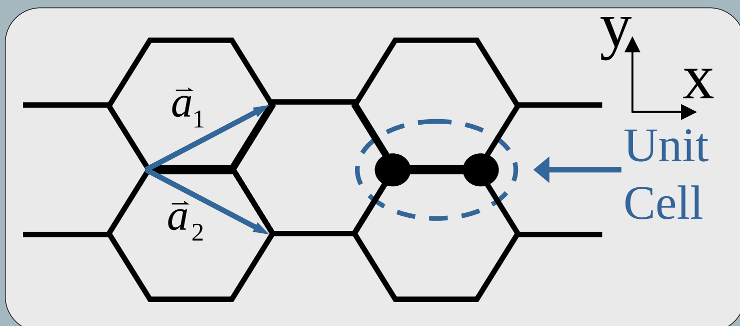
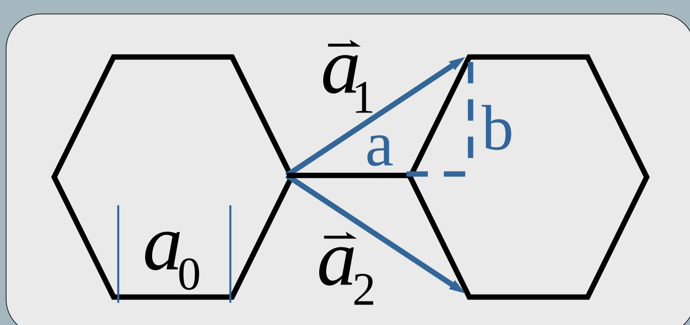
## Graphene




- Next we'd like to find DOS for a Carbon Nanotube rolled up in the y direction.




- Remember the circumferential vector:

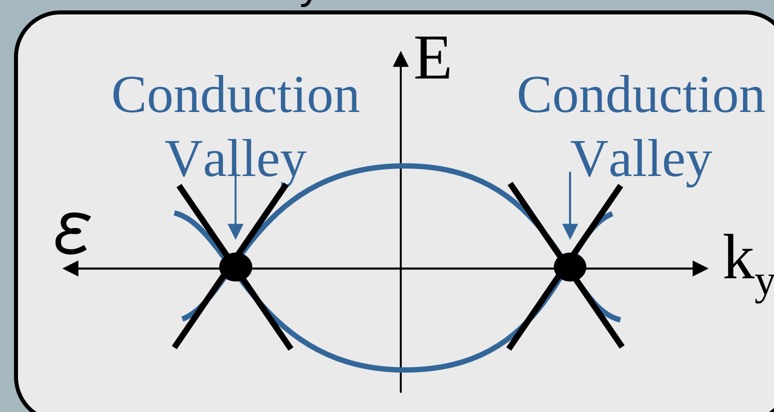
$$\boxed{c = \pi d = 2\pi m}$$

- The dispersion relation for Graphene can be written as:

$$E(k_x, k_y) \cong E_0 \pm \frac{3ta_0}{2}\sqrt{k_x^2 + \beta_y^2}$$

$$\text{where } \beta_y = k_y \pm \left(2\pi/3b\right)$$

- Remember the approximation close to conduction valleys:




- Rolling up in y direction gives the condition

$$\vec{k} \cdot \vec{C} = k_y 2mb = 2\pi\nu \Rightarrow E_\upsilon(k_x) = \ldots$$

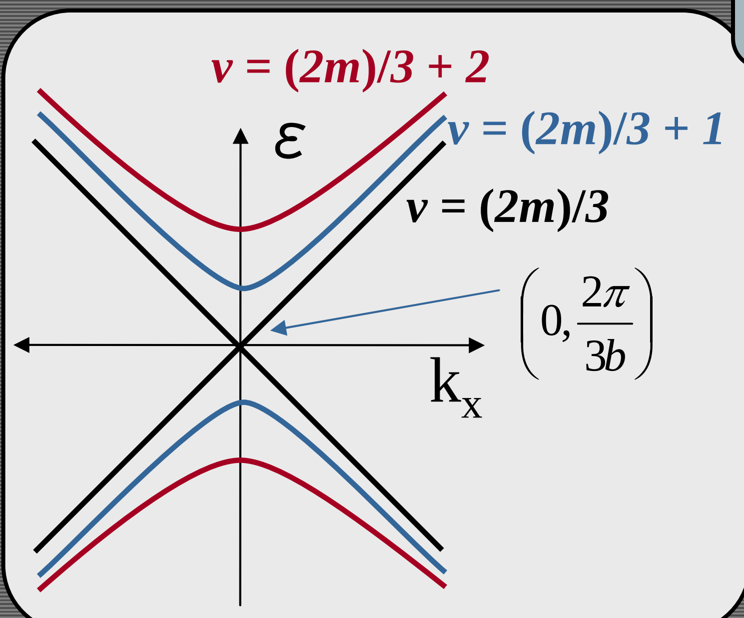
# Nanotube
# E-k / DOS



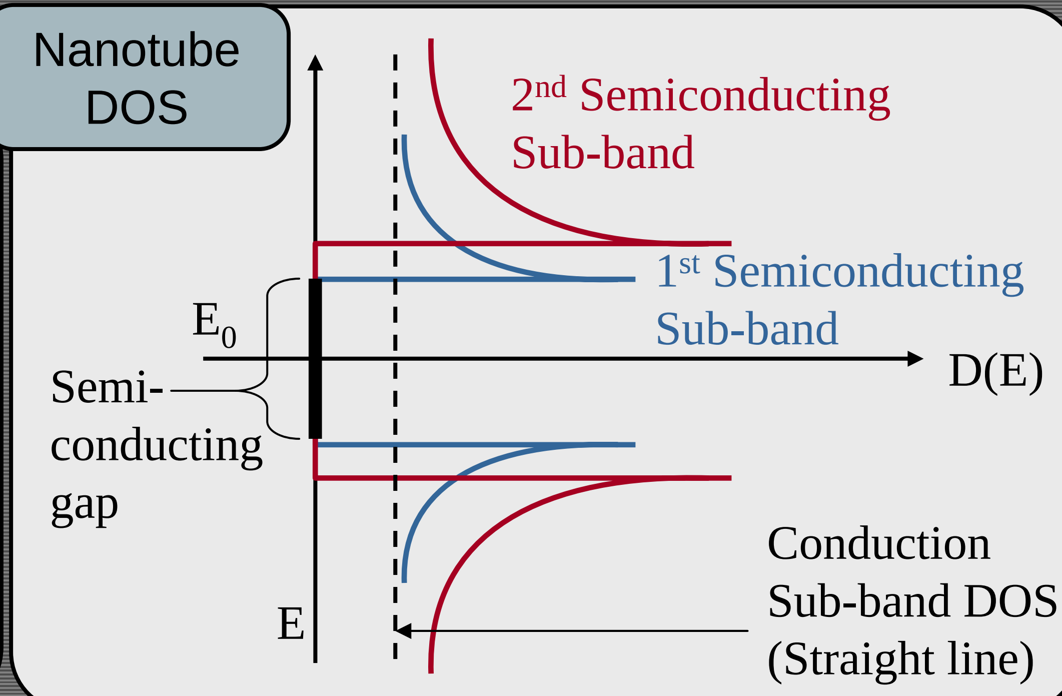
- $$E(k_x,k_y)\cong E_0 \pm \frac{3ta_0}{2}\sqrt{k_x^2+\left(k_y-\frac{2\pi}{3b}\right)^2}$$

$$\boxed{D_{1D}(E)=\frac{1}{\pi\, d\varepsilon/dk}}$$

- $$\varepsilon_\upsilon(k_x)=E_0 \pm \frac{3a_0}{2}t\sqrt{k_x^2+k_\upsilon^2} \quad \text{where } k_\upsilon \equiv \frac{2\pi\upsilon}{2bm}-\frac{2\pi}{3b}=\frac{2\pi}{2mb}\left(\upsilon-\frac{2m}{3}\right)$$




## Nanotube DOS



# Nanotube: DOS

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$$\boxed{\varepsilon_\upsilon(k_x) = \pm at\sqrt{k_x^2 + k_\upsilon^2}}$$

$$\boxed{D_{1D}(E) = \frac{1}{\pi d\varepsilon / dk}}$$

$$D(E) = \sum_\alpha \delta(E - \varepsilon_\alpha) = \sum_\upsilon \boxed{\sum_k \delta\left(E - \varepsilon_\upsilon(k)\right)} = \sum_\upsilon \frac{1}{\pi\, d\varepsilon_\upsilon / dk}$$

$$\frac{d\varepsilon_\upsilon}{dk} = at\frac{2k}{2\sqrt{k^2 + k_\upsilon^2}} = at\frac{\sqrt{E^2 - a^2t^2k_\upsilon^2}}{E}$$

$$\varepsilon = at\sqrt{k^2 + k_\upsilon^2} \Rightarrow \boxed{\varepsilon^2 - (at)^2 k_\upsilon^2 = (at)^2 k^2}$$

$$\boxed{a = \frac{3a_0}{2}}$$

$$\boxed{D(E) = \sum_\upsilon \frac{1}{\pi at}\frac{E}{\sqrt{E^2 - a^2t^2k_v^2}}}$$

# Nanotube: DOS

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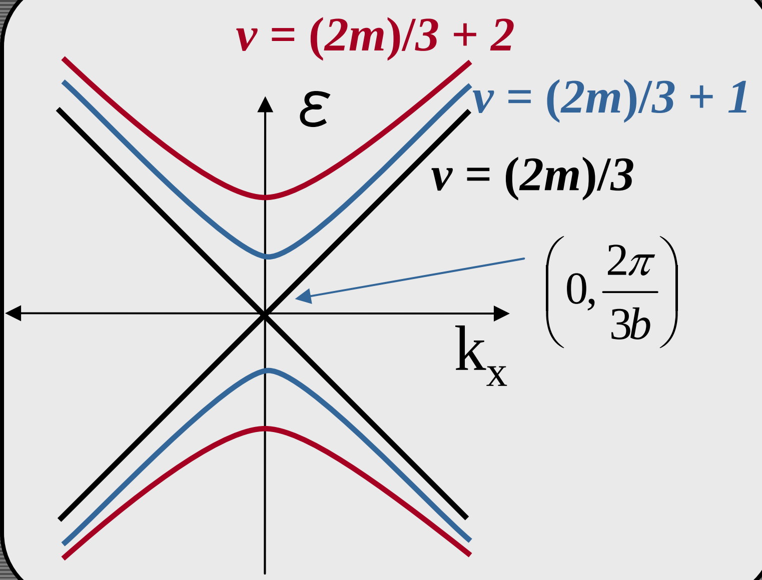
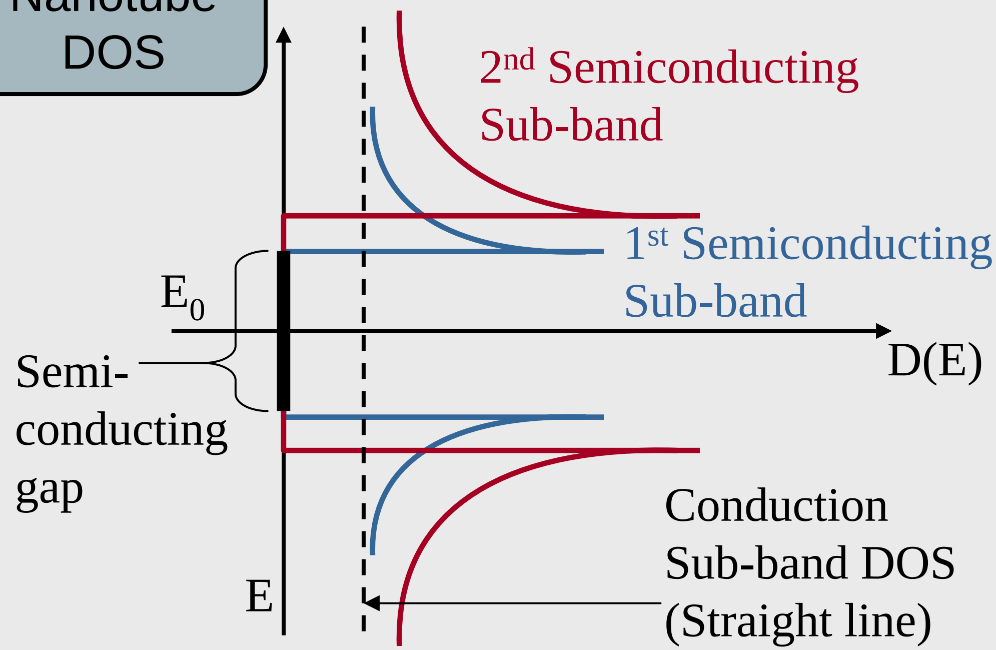
$$D(E) = \sum_{\upsilon} \frac{1}{\pi a t} \frac{E}{\sqrt{E^2 - a^2 t^2 k_v^2}}$$




Nanotube DOS

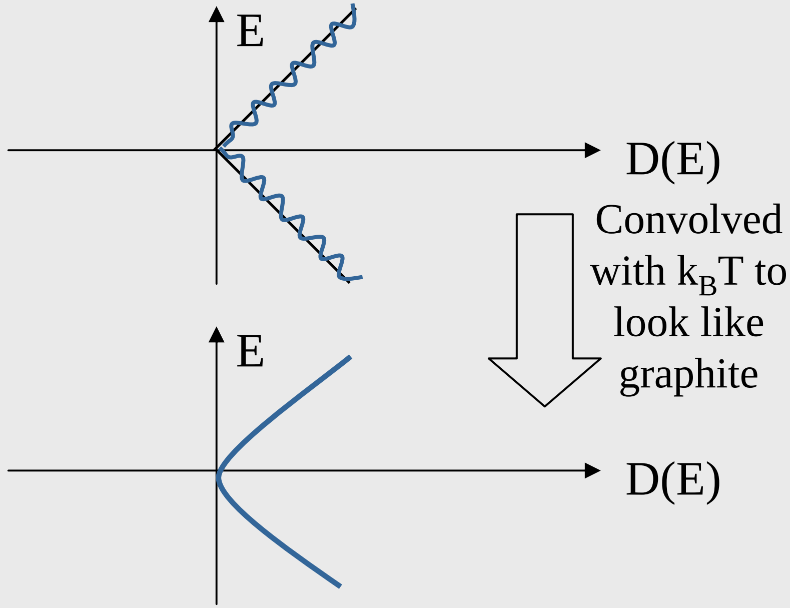


# Big Nanotubes



- The semiconducting DOS gap depends on the size of a nanotube. Those with small diameters have a large gap and those with large diameters have a small gap
- Hence, nanotubes with a large diameter begin to look like graphite! This is especially true at high temperatures, the jagged appearance of D(E) is made smooth via convolution with $k_B T$

## Big Nanotube DOS




$$D(E) = \sum_{\upsilon} \frac{1}{\pi a t} \frac{E}{\sqrt{E^2 - E_\nu^2}} \qquad E_\nu^2 = a^2 t^2 k_\nu^2$$

$$k_\upsilon \equiv \frac{2\pi\upsilon}{2bm} - \frac{2\pi}{3b} = \frac{2\pi}{2mb}\left(\upsilon - \frac{2m}{3}\right)$$

$$D(E) \propto \int dE_\upsilon \frac{E}{\sqrt{E^2 - E_\upsilon^2}} = E$$

$$\boxed{dk_\upsilon = dE_\upsilon}$$