Fundamentals of Nanoelectronics

ECE495 - Session 26, Oct 28, 2009

Reciprocal Lattice

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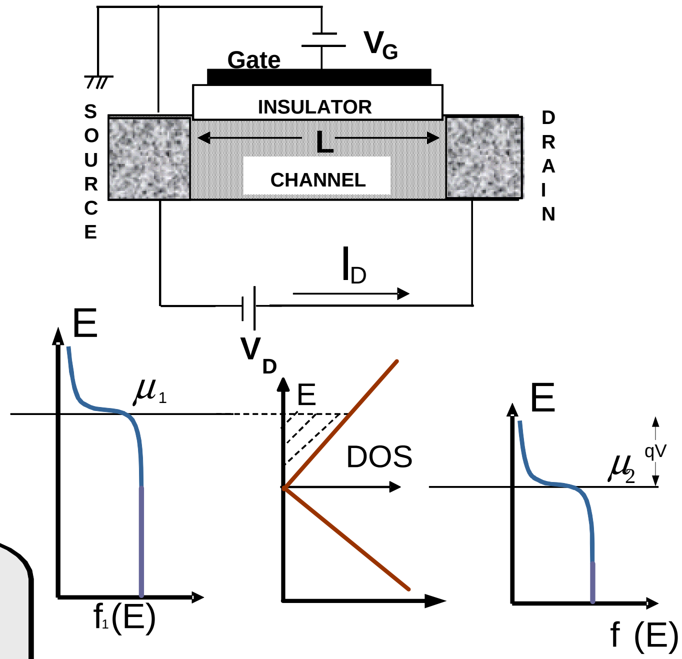
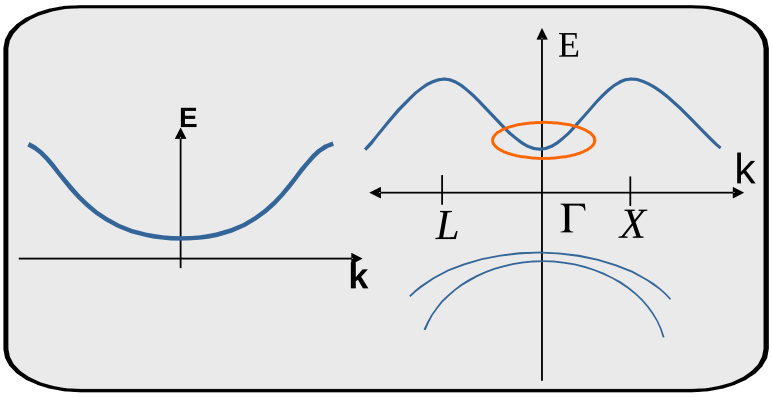
Review

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

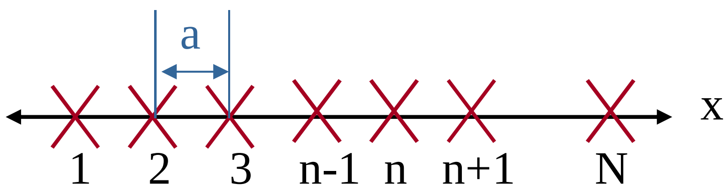
$$N = \int dE\,\frac{D(E)}{2}\left(f_1(E) - f_2(E)\right)$$

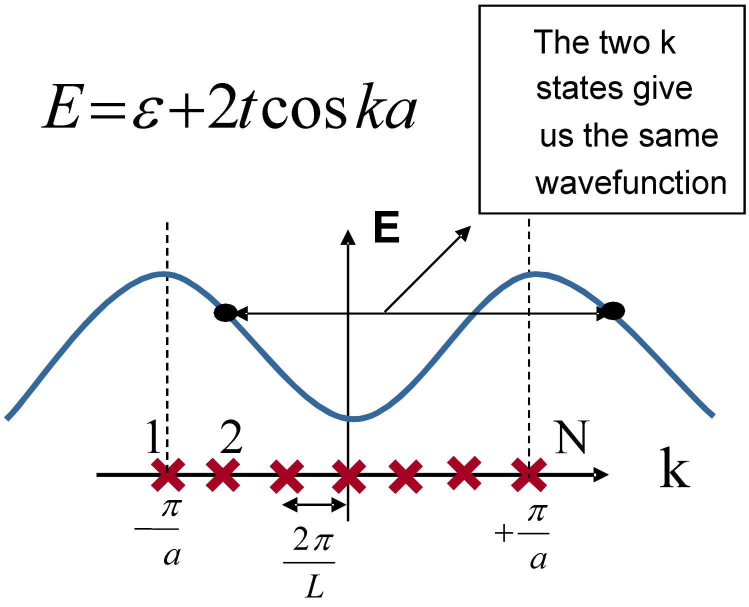




One Dimensional Lattice

Given any periodic structure we've discussed how to calculate the E-k relationship. For example consider a 1-D solid:





The number of allowed values of k can be found as:

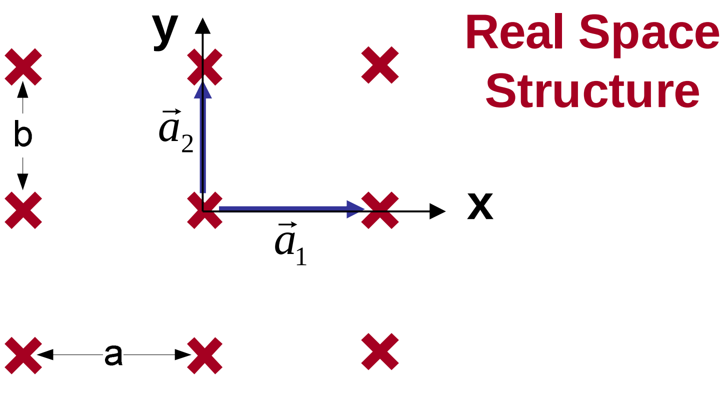
$$\frac{2\pi/a}{2\pi/L}=\frac{L}{a}=N$$

The point is that if you take any value of k within the range and add 2π/a to it, you will not get a new independent wavefunction.

$\psi_n=\underbrace{\psi_0 e^{ikna}e^{i2\pi n}}_{1}=\underbrace{\psi_0 e^{ikna}}_{2}$ You can clearly see that 1 and 2 are the same. This is why we do not need to consider any k values outside of the range –π/a and π/a. The point is that corresponding to any point outside the range there is a point within the range which is an integer multiple of 2π/a from it. It is the same story for all of them. Add this amount to k and you will get the same answer.

This symmetric interval around k=0 states that gives us a complete set of k values is called the first ***Brillouin zone***.

Two Dimensional Lattice



Any point in the real space can be written as:

$$\vec{r}=n\underbrace{\hat{x}a}_{\vec{a}_1}+m\underbrace{\hat{y}b}_{\vec{a}_2}=n\vec{a}_1+m\vec{a}_2$$

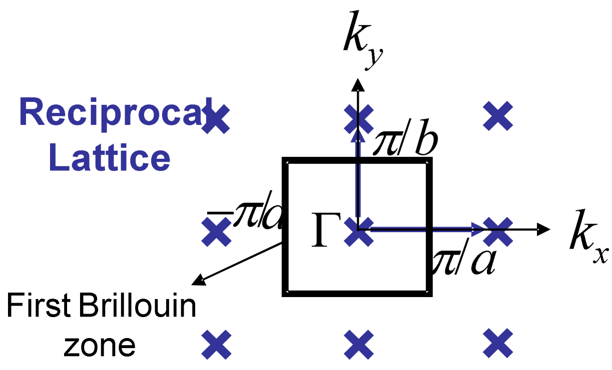
where n and m are integers.

Where the general solution is:

$$\psi(\vec{r})=\psi_0 e^{i\vec{k}\cdot\vec{r}}$$

To construct the reciprocal lattice we need to find a vector ***K*** such that:

$$e^{i(\vec{k}+\vec{K})\cdot\vec{r}}=e^{i\vec{k}\cdot\vec{r}}\Rightarrow e^{i\vec{K}\cdot\vec{r}}=1\Rightarrow\vec{K}\cdot\vec{r}=(2\pi)\upsilon$$



Any point in the reciprocal lattice can be written as: $\vec{K} = M\vec{A}_1 + N\vec{A}_2$

To find K the general procedure is to find the vectors A1 and A2 that satisfy:

$$\begin{aligned} \vec{a}_1 \cdot \vec{A}_1 = \vec{a}_2 \cdot \vec{A}_2 = 2\pi \\ \vec{a}_1 \cdot \vec{A}_2 = \vec{a}_2 \cdot \vec{A}_1 = 0 \end{aligned} \Rightarrow \begin{aligned} \vec{A}_1 = \hat{x}(2\pi/a) \\ \vec{A}_2 = \hat{y}(2\pi/a) \end{aligned}$$

We can now check to see if we have the right answer:

$$\vec{K}\cdot\vec{r} = \quad (m\hat{x}a + n\hat{y}a) \quad \cdot(\hat{x}\frac{2\pi}{a} + \hat{y}\frac{2\pi}{a})$$

$$= 2\pi(Mm + Nn)$$

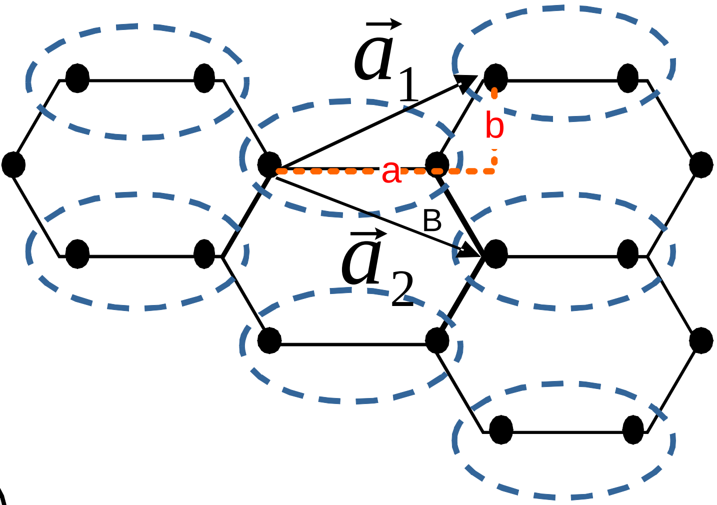
Graphene Brollouin Zoon

$\overrightarrow{A_1} = \frac{2\pi.(\overrightarrow{a_2}\times\overrightarrow{a_3})}{\overrightarrow{a_1}.(\overrightarrow{a_2}\times\overrightarrow{a_3})}$ and $\overrightarrow{A_2} = \frac{2\pi.(\overrightarrow{a_1}\times\overrightarrow{a_3})}{\overrightarrow{a_2}.(\overrightarrow{a_1}\times\overrightarrow{a_3})}$ where $\vec{a}_1 = a\hat{x} + b\hat{y}$,$\vec{a}_2 = a\hat{x} - b\hat{y}$ *and* $\vec{a}_3 = c\hat{z}$

Hence substituting a_1, a_2 and a_3 to A_1 and A_2 we have:

$$\overrightarrow{A_1} = \frac{2\pi.(-\hat{x}b - \hat{y}a)c}{-2abc} \Rightarrow \overrightarrow{A_1} = \hat{x}\frac{\pi}{a} + \hat{y}\frac{\pi}{b}$$

$$\overrightarrow{A_2} = \frac{2\pi.(-\hat{x}b + \hat{y}a)c}{-2abc} \Rightarrow \overrightarrow{A_1} = \hat{x}\frac{\pi}{a} - \hat{y}\frac{\pi}{b}$$



$$\varepsilon(\vec{k}) = \pm a\sqrt{k_x^2 + k_y^2}$$