Reference book:

# Quantum Transport

## Atom to Transistor

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Cambridge University Press, 2005

## Wave in a 1D line:

**wave equation** $\boxed{\dfrac{\partial^2 u}{\partial t^2} = v^2 \dfrac{\partial^2 u}{\partial x^2}}$

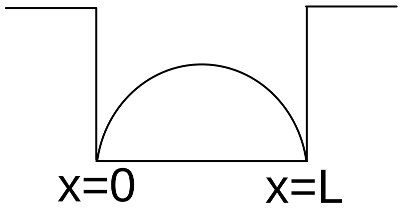
**Solution: plan wave** $u = u_0 \exp(kx)\exp(-i\omega t) \Rightarrow \omega^2 = v^2 k^2 \Rightarrow \omega = \pm vk$ **Linear dispersion**

With the 2 ends fixed, ***i.e. u*(0)=0; *u*(L)=0 :**

$$u = u_0 \sin(kx)\exp(-i\omega t) \Rightarrow k = n\pi / L \Rightarrow \omega = n\pi v / L$$

**Discrete *k* values due to confinement**

## In 1D Schrödinger equation:



$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

**Solution: plan wave**

$$\Psi = \Psi_0 \exp(ikx)\exp(-iEt/\hbar) \Rightarrow E = \frac{\hbar^2 k^2}{2m}$$ **parabolic dispersion**

With the 2 ends fixed, ***i.e. u*(0)=0; *u*(L)=0 :**

$$\Psi = \Psi_0 \sin(kx)\exp(-iEt/\hbar) \Rightarrow k = n\pi / L$$

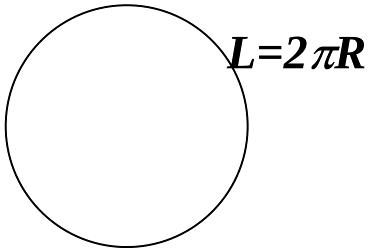
$$\Rightarrow E = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

**Ch. 2.1, p.35, 36**

# Standing waves in a ring: periodic boundary condition

$$\left.\begin{aligned}\Psi &= \Psi_0 \sin(kx)\exp(-iEt/\hbar) \\ \Psi &= \Psi_0 \cos(kx)\exp(-iEt/\hbar)\end{aligned}\right\}$$ Degenerate states

$$k = 2n\pi / L \Rightarrow E = \frac{2\hbar^2\pi^2 n^2}{mL^2}$$



standing waves in a ring

## Compared with the wavefunction in a linear line:

1. **Spacing between k values = 2π/L instead of π/L**
2. **Existence of degenerate states**

## the wave functions can also be expressed as

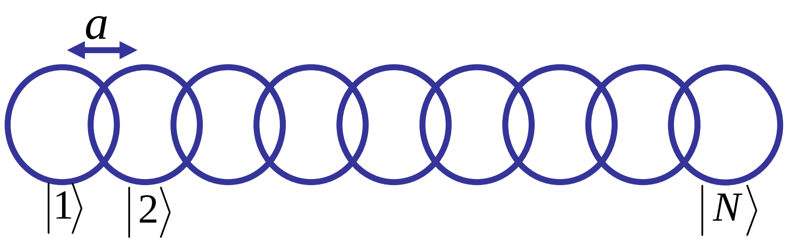
$$\Psi = \Psi_0 \exp(+ikx)\exp(-iEt/\hbar)$$ traveling in +x direction

$$\Psi = \Psi_0 \exp(-ikx)\exp(-iEt/\hbar)$$ traveling in -x direction

$$k = 2n\pi / L \Rightarrow E = \frac{2\hbar^2\pi^2 n^2}{mL^2}$$

**Ch. 2.1, p.37**

# A 1D crystal



$$E\psi = H\psi$$

$$H = \begin{array}{c|cccccc} & |1\rangle & |2\rangle & \cdots & \cdots & |N-1\rangle & |N\rangle \\ \hline |1\rangle & E_0 & E_{SS} & & & 0 & E_{SS} \\ |2\rangle & E_{SS} & E_0 & & & 0 & 0 \\ & & & \cdots & \cdots & \cdots & \\ & & & \cdots & \cdots & \cdots & \\ |N-1\rangle & 0 & 0 & & & E_0 & E_{SS} \\ |N\rangle & E_{SS} & 0 & \cdots & \cdots & E_{SS} & E_0 \end{array}$$

**wrapping**

**Inter-orbital coupling (overlap integral)**

**self-energy**

$$E\psi_n = E_0\psi_n + E_{SS}\psi_{n-1} + E_{SS}\psi_{n+1} \qquad n=1,\ 2,\ \ldots,\ N$$

ansatz: $\psi_n = \psi_0 e^{ikna}$

$$E\psi_0 = E_0\psi_0 + E_{SS}e^{-ika}\psi_0 + E_{SS}e^{+ika}\psi_0$$

$$\Rightarrow E = E_0 + 2E_{SS}\cos(ka)$$

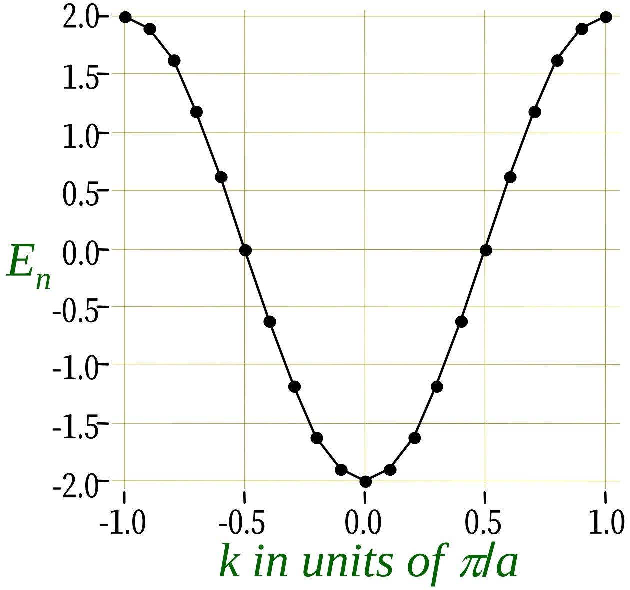
$$E_n = E_0 + 2E_{SS}\cos(k_n a) \quad \text{where} \quad k_n a = 2n\pi / N$$

**# of eigenvalues = *n*** (it is finite due to finite lattice size)

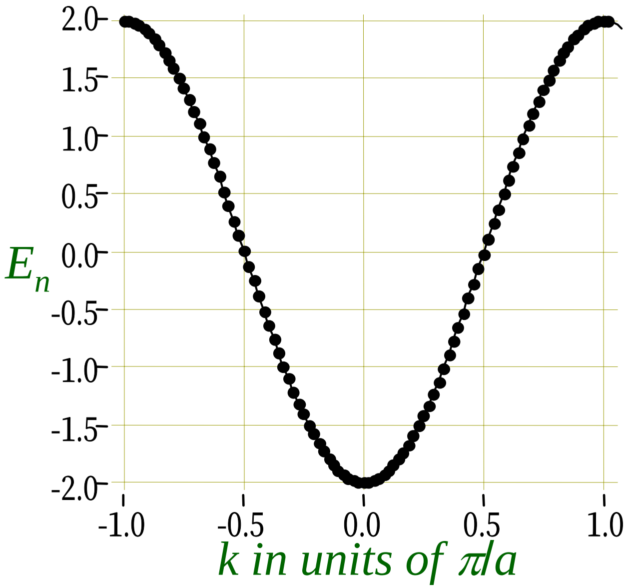
**Ch. 5.1, p.105**

# Plots of eigenvalues in a unit cell (Brillouin zone)

$$E_n = E_0 + 2E_{SS}\cos\left(k_n a\right) \quad \text{where} \quad k_n a = 2n\pi / N$$



$E_0$=0, $E_{SS}$=-1, $N$=20



$E_0$=0, $E_{SS}$=-1, $N$=100

Discrete allowed ***k*** values (in units of $2\pi/Na$) due to finite range of lattice (=$Na$)

Discrete lattice ($a$) leads to finite range of allowed $k$ (=$2\pi/a$)

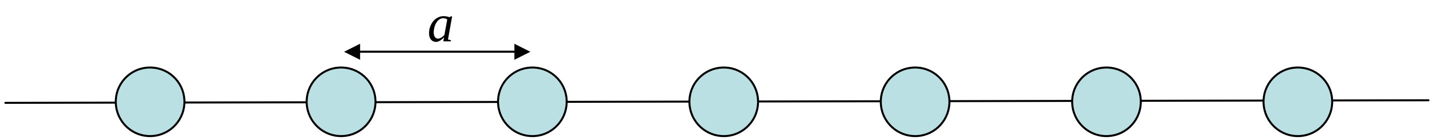
# of atoms (unit cells) in real space = # of eigenvalues = # of allowed $k$ values
= size of the matrix [$H$]

For **s** coupling, $E_{SS}$<0 (upward) ; for ***p*** coupling, $E_{SS}$>0 (downward)

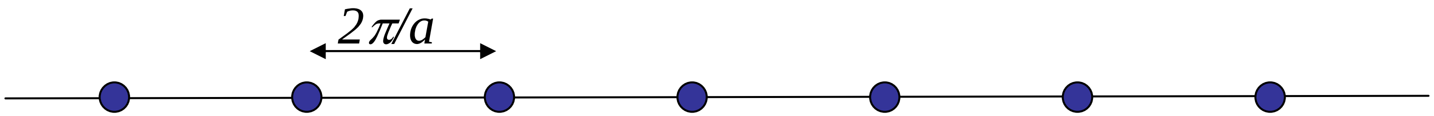
**Ch. 5.1, p.106, 107**

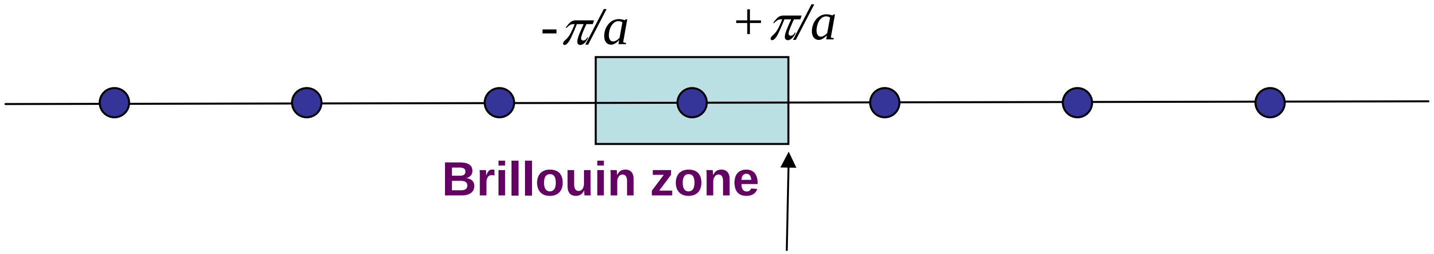
# Brillouin zone for 1D

**Direct lattice**



**Reciprocal lattice**



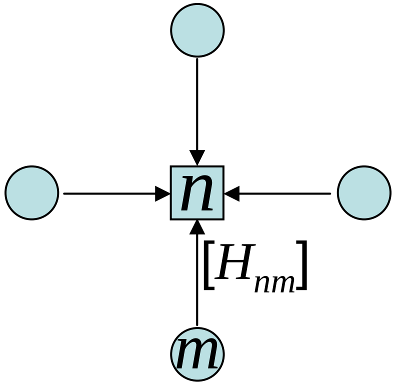


**Brillouin zone**

**bisector**

**Ch. 5.2, p.112**

# Band structure of a 2D system



$$\sum_m [H_{nm}]\{\phi_m\} = E\{\phi_n\}$$

matrix size = ($b\times b$), $b$=# of basis functions per cell.
vector size = ($b\times 1$)

Ansatz: $\{\phi_m\} = \{\phi_0\} e^{i\vec{k}\cdot\vec{d}_m}$

$$\sum_m [H_{nm}]\{\phi_m\} = \sum_m [H_{nm}] e^{i\vec{k}\cdot\vec{d}_m}\{\phi_0\} = E e^{i\vec{k}\cdot\vec{d}_n}\{\phi_0\}$$

$$E\{\phi_0\} = \sum_m [H_{nm}] e^{i\vec{k}\cdot(\vec{d}_m-\vec{d}_n)}\{\phi_0\} \equiv [h(\vec{k})]\{\phi_0\}$$

Dispersion curves = the eigenvalues of the ($b\times b$) matrix $[h(\vec{k})]$ for each $k$ value

totally $b$ branches

Ch. 5.2, p.110

# Allowed values of *k*:

$$\left[\vec{k}\right]_{mn} = \hat{x}(m\,2\pi/Ma) + \hat{y}(n\,2\pi/Nb)$$

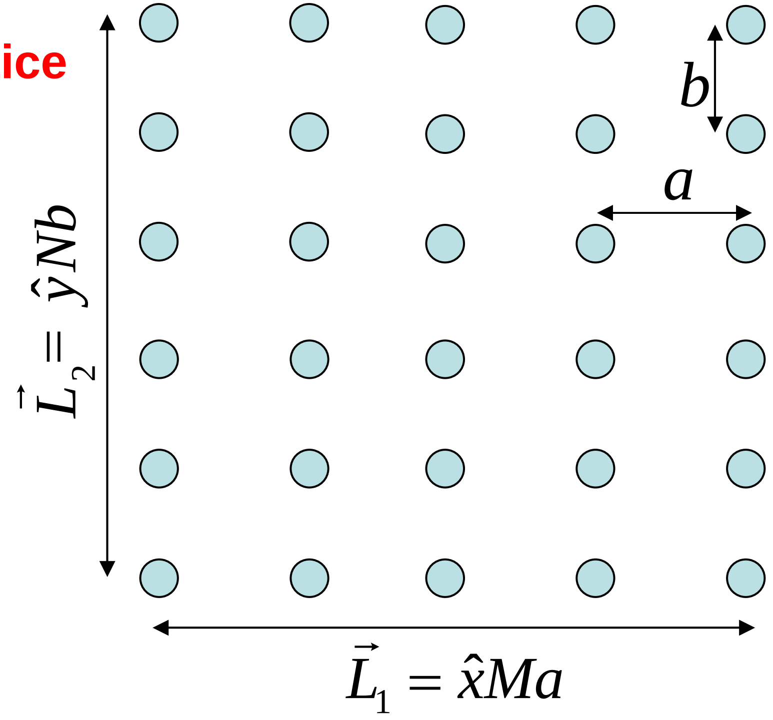
$m$, $n$ are integers

c.f. for 1D crystal $k_n = 2n\pi / Na$

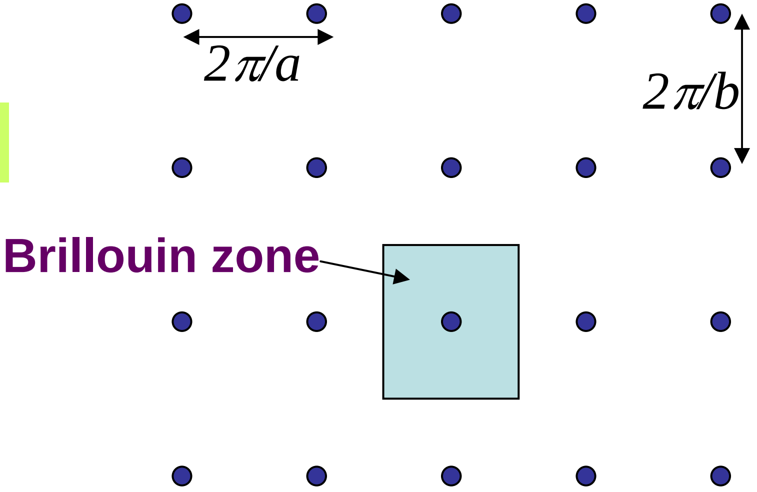
**Brillouin zone for 2D**

In the Brillouin zone, $m \le M$ and $n \le N$

**Direct lattice**



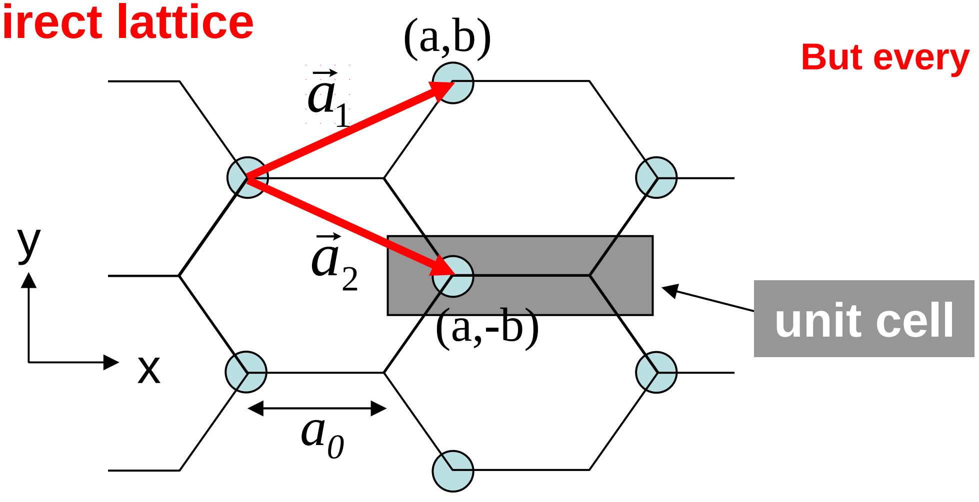
**Reciprocal lattice**



**Ch. 5.2, p.111, 112**

# Graphite sheet (graphene layer)

**Direct lattice**



Adjacent atoms do not have the same environment

But every **unit cell** has identical environment:
a periodic condition

$$\vec{c} = m\vec{a}_1 + n\vec{a}_2$$

$\vec{a}_1$ **and** $\vec{a}_2$ are basis vectors

$$a \equiv 3a_0/2 \qquad b \equiv \sqrt{3}a_0/2$$

$$\vec{a}_1 \equiv \hat{x}a + \hat{y}b \qquad \vec{a}_2 \equiv \hat{x}a - \hat{y}b$$

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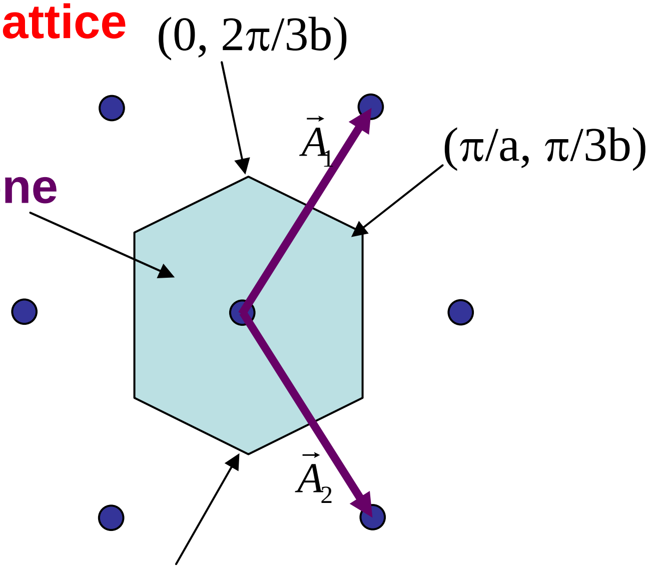
**Reciprocal lattice**



**Brillouin zone**

**Perpendicular bisector**

$$\vec{K} = M\vec{A}_1 + N\vec{A}_2$$

$$\boxed{\vec{A}_1 \cdot \vec{a}_1 = 2\pi} \qquad \boxed{\vec{A}_2 \cdot \vec{a}_2 = 2\pi}$$

$$\vec{A}_1 = \frac{2\pi(\vec{a}_2 \times \hat{z})}{\vec{a}_1 \cdot (\vec{a}_2 \times \hat{z})} = \hat{x}\left(\frac{\pi}{a}\right) + \hat{y}\left(\frac{\pi}{b}\right)$$

$$\vec{A}_2 = \frac{2\pi(\hat{z} \times \vec{a}_1)}{\vec{a}_2 \cdot (\hat{z} \times \vec{a}_1)} = \hat{x}\left(\frac{\pi}{a}\right) - \hat{y}\left(\frac{\pi}{b}\right)$$

$$\boxed{\vec{A}_1 \perp \vec{a}_2} \qquad \boxed{\vec{A}_2 \perp \vec{a}_1}$$

Ch. 5.2, p.114

# Two basis functions

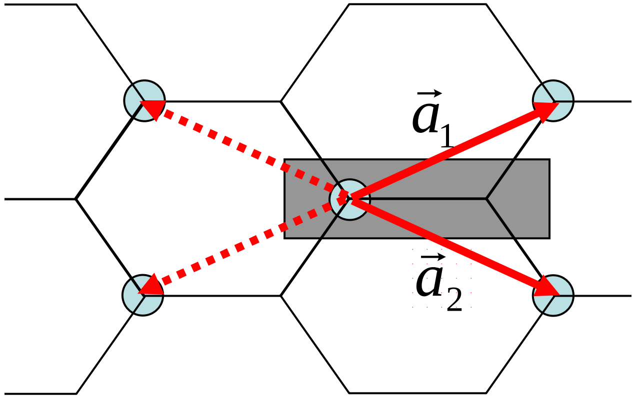
For graphene, the levels involving $2s$, $2p_x$, $2p_y$ orbits are either far above or far below the Fermi level

The conduction and valence band levels are essentially formed out of the $2P_z$ orbits.

One $2P_z$ orbital per carbon atom and two atoms per unit cell → two basis functions

$$E\{\phi_0\} = \sum_m [H_{nm}]\, e^{i\vec{k}\cdot(\vec{d}_m-\vec{d}_n)}\{\phi_0\} \equiv [h(\vec{k})]\{\phi_0\}$$

**Direct lattice**



$$[h(\vec{k})] = \begin{bmatrix} 0 & -t \\ -t & 0 \end{bmatrix} + \begin{bmatrix} 0 & -t\exp(i\vec{k}\cdot\vec{a}_1) \\ 0 & 0 \end{bmatrix} + \begin{bmatrix} 0 & -t\exp(i\vec{k}\cdot\vec{a}_2) \\ 0 & 0 \end{bmatrix}$$

$$+ \begin{bmatrix} 0 & 0 \\ -t\exp(-i\vec{k}\cdot\vec{a}_1) & 0 \end{bmatrix} + \begin{bmatrix} 0 & 0 \\ -t\exp(-i\vec{k}\cdot\vec{a}_2) & 0 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & -t(1+e^{i\vec{k}\cdot\vec{a}_1}+e^{i\vec{k}\cdot\vec{a}_2}) \\ -t(1+e^{-i\vec{k}\cdot\vec{a}_1}+e^{-i\vec{k}\cdot\vec{a}_2}) & 0 \end{bmatrix}$$

$$\equiv \begin{bmatrix} 0 & h_0 \\ h_0^* & 0 \end{bmatrix}$$

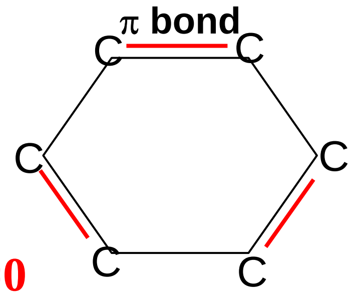
$$h_0 \equiv -t(1+e^{i\vec{k}\cdot\vec{a}_1}+e^{i\vec{k}\cdot\vec{a}_2}) = -t(1+2\exp(ik_x a)\cos k_y b)$$

$$E = \pm|h_0| = \pm t\sqrt{1+4\cos k_y b\cos k_x a + 4\cos^2 k_y b}$$

**Ch. 5.2, p.115**

# Energy band

2 basis function per cell → total # of states = $2N$, $N$ = # of unit cells

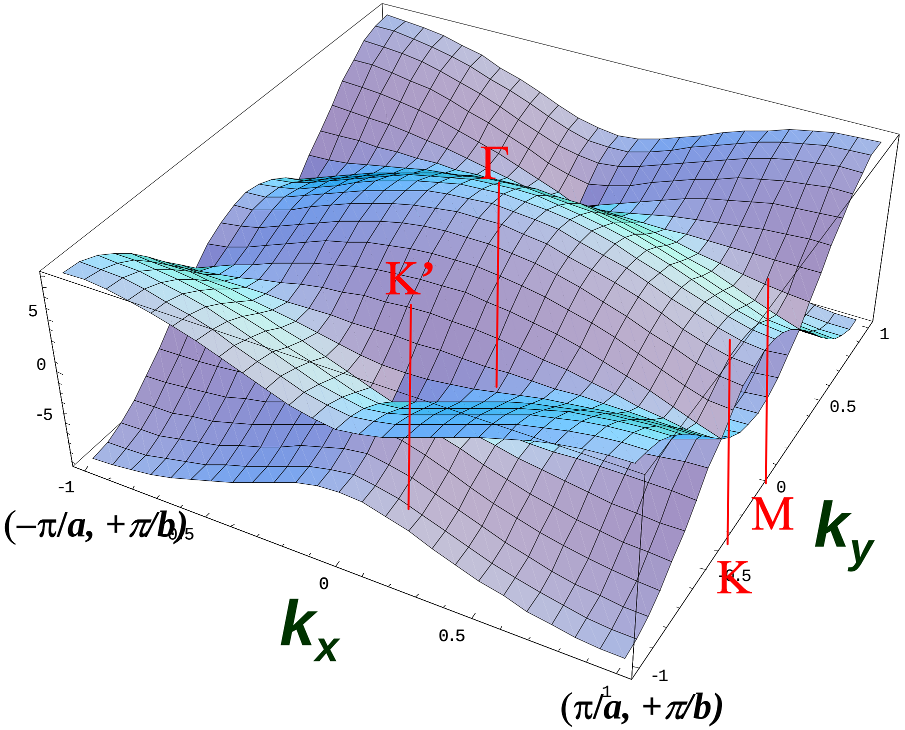


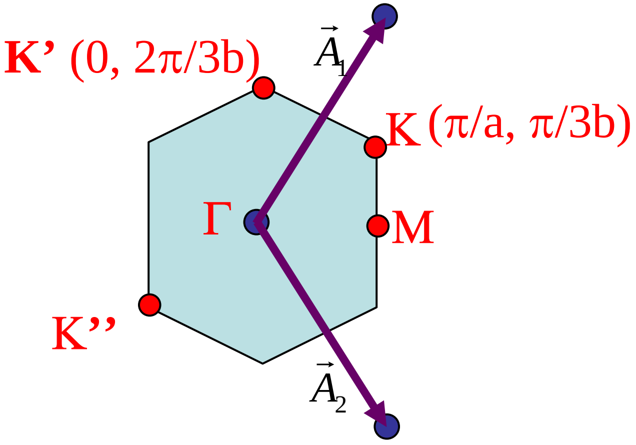
2 atoms per cell, each atom contribute 1 electron, total $2N$ electrons
→ **fill up half of states**.

Energy levels: symmetrical about $\boldsymbol{E}$ **=0** → **Fermi level** is located at $\boldsymbol{E}$**=0**

$$h_0 \equiv -t(1+e^{i\vec{k}\cdot\vec{a}_1}+e^{i\vec{k}\cdot\vec{a}_2}) = -t(1+2\exp(ik_xa)\cos k_yb)$$

$$E=\pm|h_0| = \pm t\sqrt{1+4\cos k_yb\cos k_xa+4\cos^2 k_yb}$$





$$E=0 \to h_0(\vec{k})=0$$

$$\exp(ik_xa)\cos k_yb=-1/2$$

**K':** $k_xa=0,\quad k_yb=\pm 2\pi/3$

**K:** $k_xa=\pi,\quad k_yb=\pm\pi/3$

$k_xa=-\pi,\quad k_yb=\mp 2\pi/3$

**Ch. 6.1, p.133**

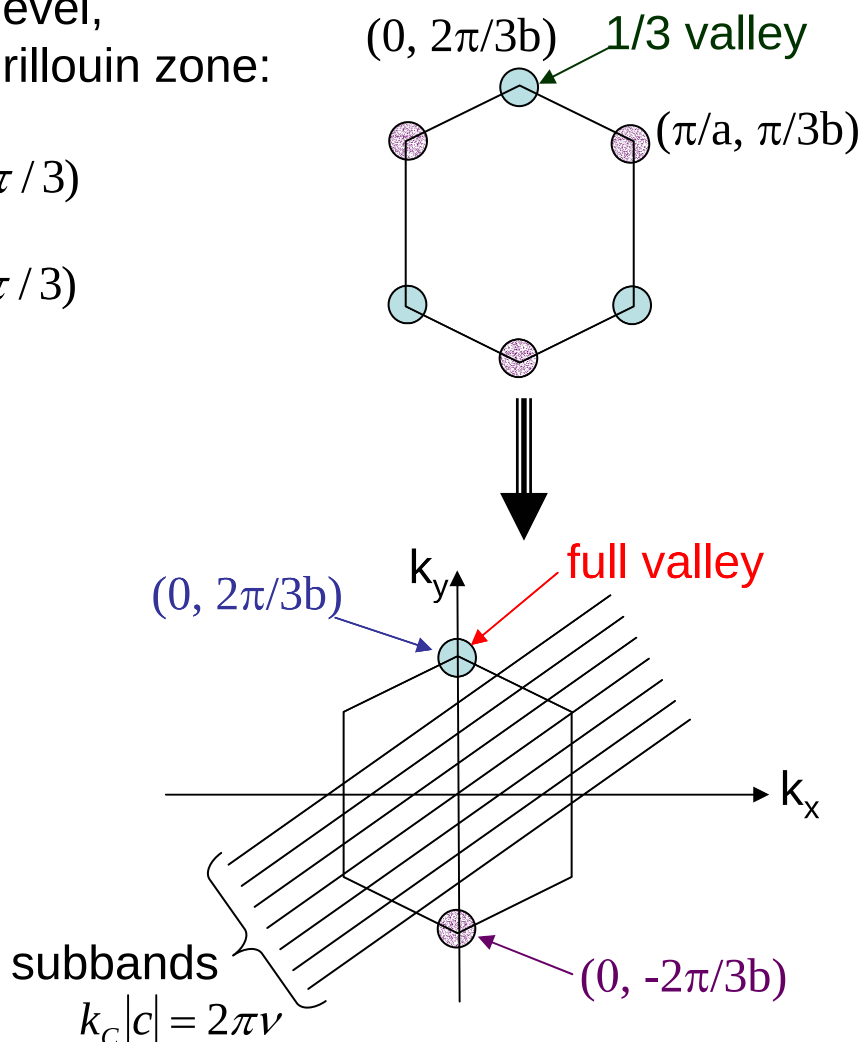
# From Graphene to Carbon nanotube

Two groups of three points around the Fermi level,
each contains 1/3 of a valley in 1st Brillouin zone:

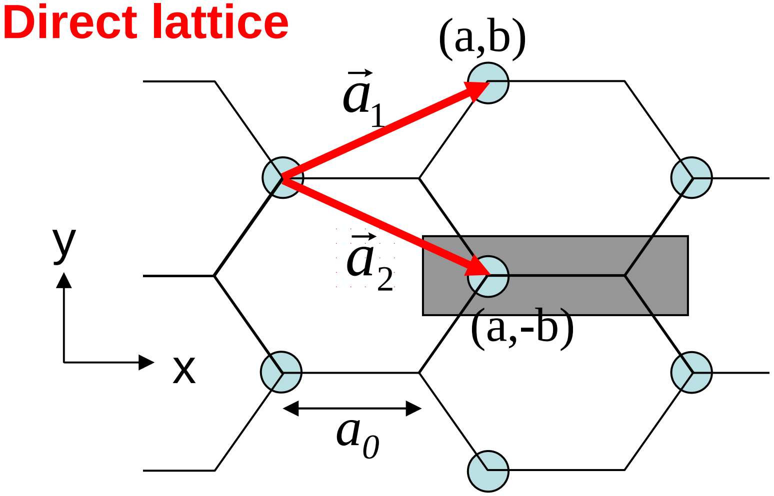
$$\begin{array}{l} (k_x a, k_Y a) = \\[1em] (k_x a, k_Y a) = \end{array} \boxed{\begin{array}{l} (0,+2\pi/3), \\[1em] (0,-2\pi/3), \end{array}} \; \begin{array}{ll} (-\pi,-2\pi/3), & (+\pi,-\pi/3) \\[1em] (-\pi,+2\pi/3), & (+\pi,+\pi/3) \end{array}$$

full valley

## Reciprocal lattice



## Direct lattice



$$\vec{c} = m\vec{a}_1 + n\vec{a}_2 = \hat{x}(m+n)a + \hat{y}(m-n)b$$

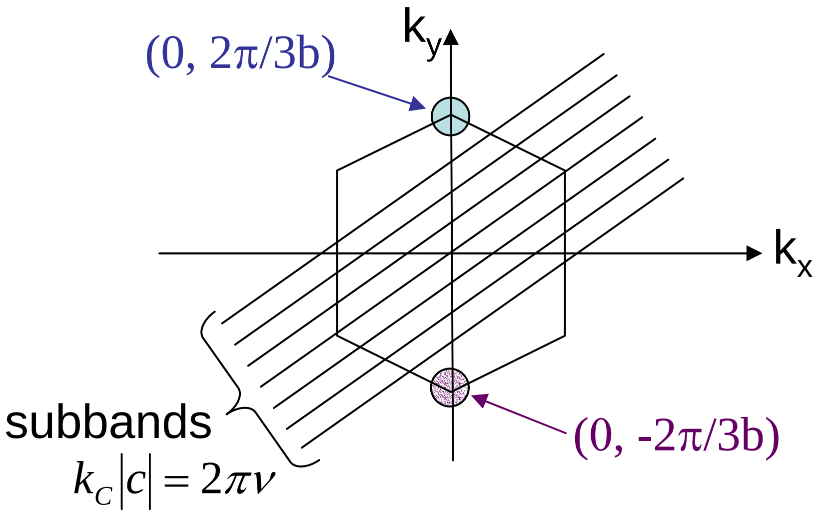
## When rolled up into a nanotube

constrained by boundary condition $\vec{k}\cdot\vec{c} \equiv k_C|c| = k_x a(m+n) + k_y b(m-n) = 2\pi\nu$

$\nu$ = integer

**Ch. 6.1, p.134**

# Metallic or Semiconductor?



Metallic: if one of the subbands passes the center of one of the valleys

Semiconductor: otherwise

$$\vec{k}\cdot\vec{c} \equiv k_C|c| = k_x a(m+n) + k_y b(m-n) = 2\pi\nu$$

to pass through (0, 2π/3b): $(m-n)/3 = \nu$

For metallic tubes: $m - n = 3\nu$

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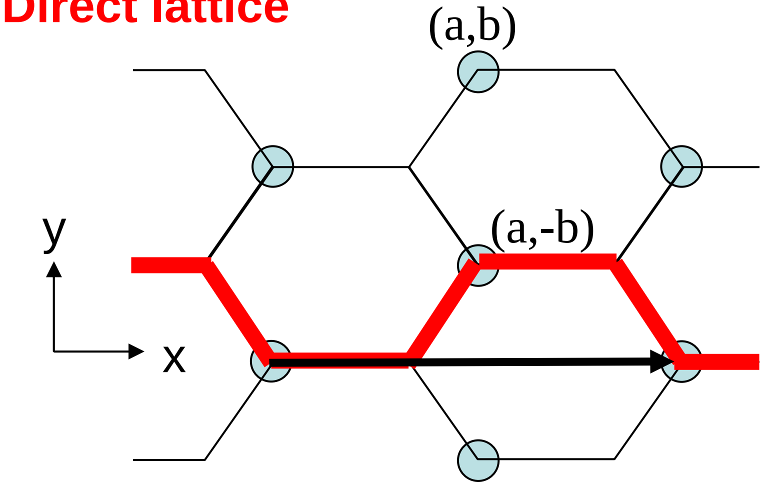
## For armchair tubes: *m = n*

**Direct lattice**



$$\vec{c} = \hat{x}2am$$

$$k_x 2am = 2\pi\nu \Rightarrow k_x = \frac{2\pi\nu}{2ma}$$

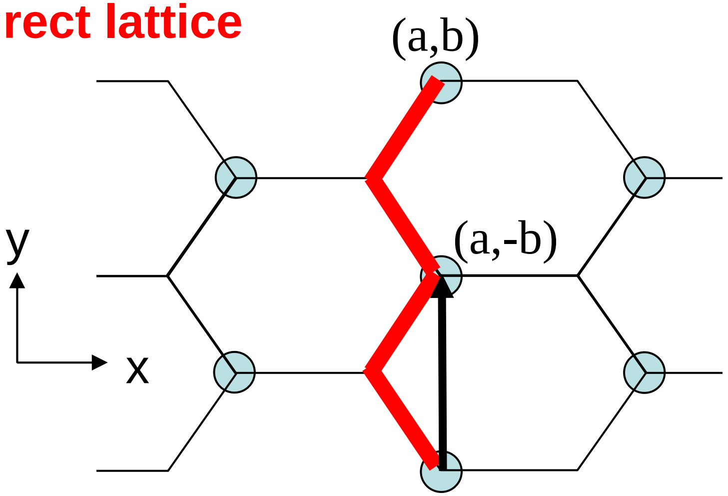
**subband with $\nu$=0 always pass $E$=0 points**

**Always metallic, regardless of *m* value**

Ch. 6.1, p.135

# For zigzag tubes:

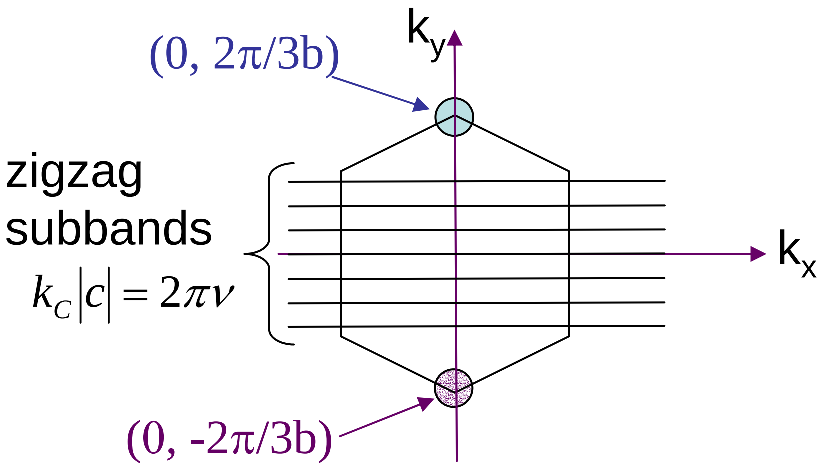
## Direct lattice



$$\vec{c} = \hat{y}2bm$$

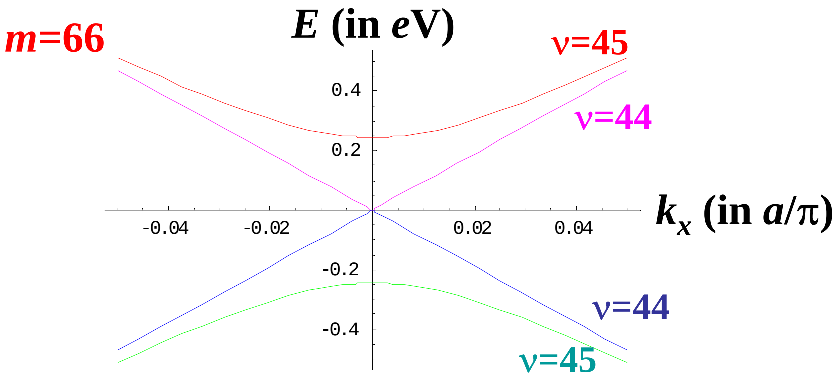
$$k_y 2bm = 2\pi\nu \Rightarrow k_y = \frac{2\pi}{3b}\frac{3\nu}{2m}$$

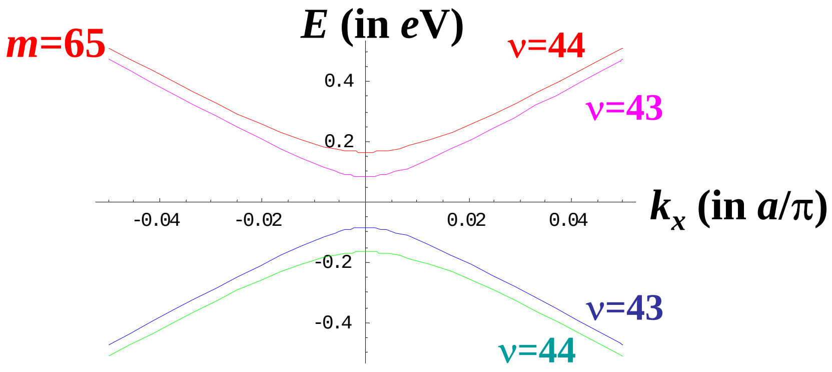
$3\nu = 2m \rightarrow$ ***m* = a multiple of 3**



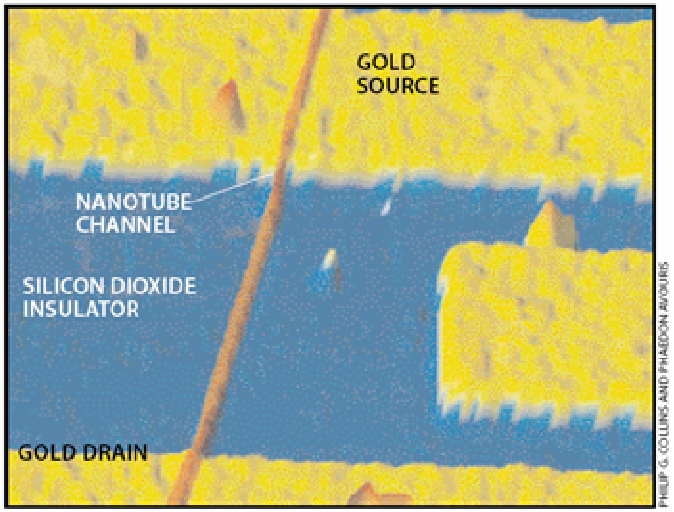
zigzag subbands

$$k_C|c| = 2\pi\nu$$

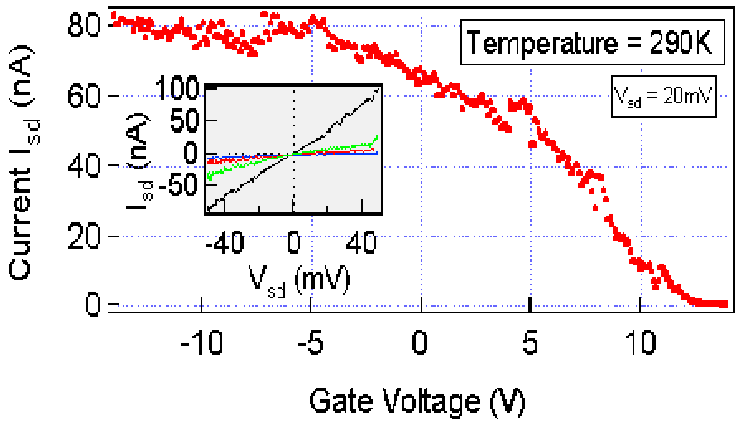


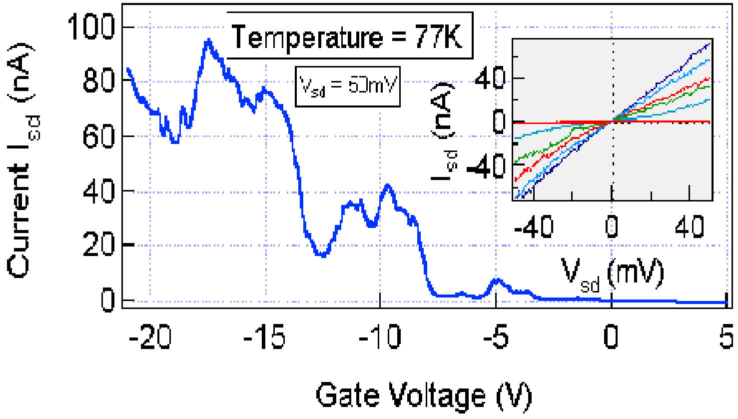


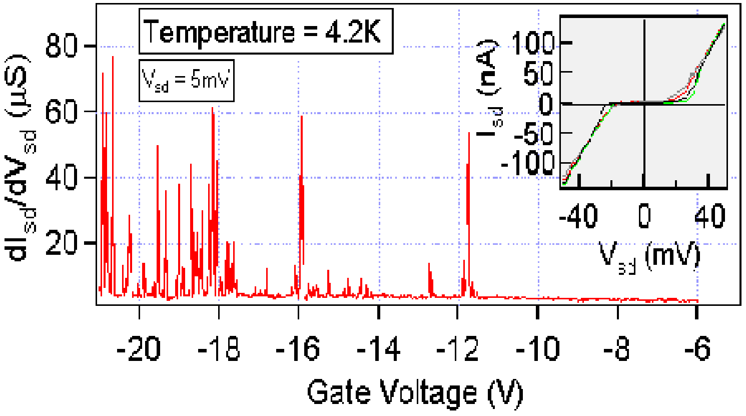
# Transition from FET to SET



**As we cool the FET down from room temperature to 4 degree Kelvin, we see the device behavior change dramatically. While the device acts like a field-effect transistor at room temperature, at 4K it behaves like a single-electron transistor (SET).**







http://www.research.ibm.com/nanoscience/fet.html