Square potential Wells

How many electrons are in a material?

$$n = \int_{-\infty}^{+\infty} g(E) f(E,\mu) dE$$

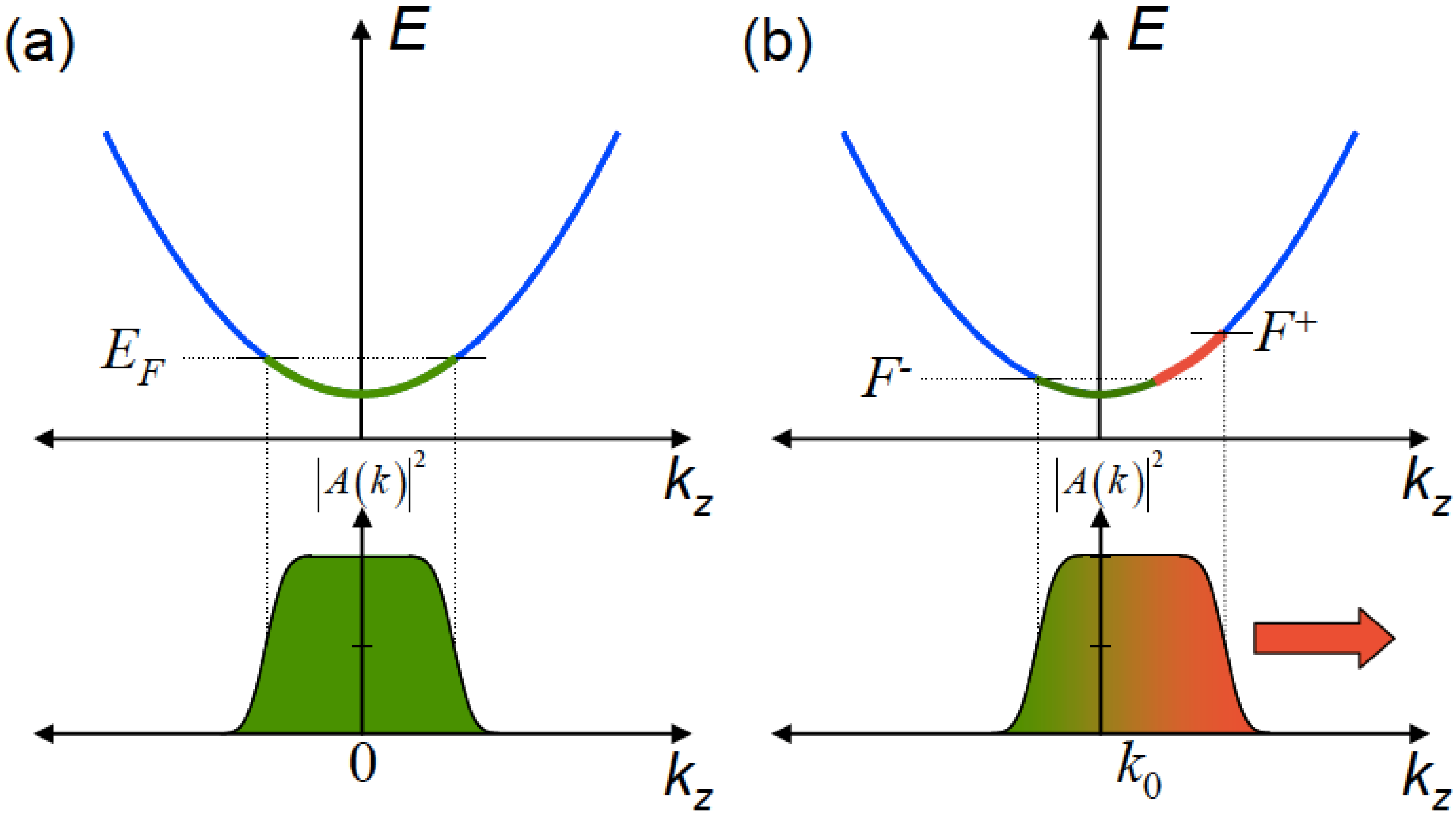
g(E): Density of states (DOS) (two electrons per state)
f(E,μ): Fermi distribution ($\mu = E_f$)

$$f(E,\mu) = \frac{1}{1 + \exp\left[(E-\mu)/kT\right]}$$

If electrons are described by plane waves then the energies that can occupy are given by

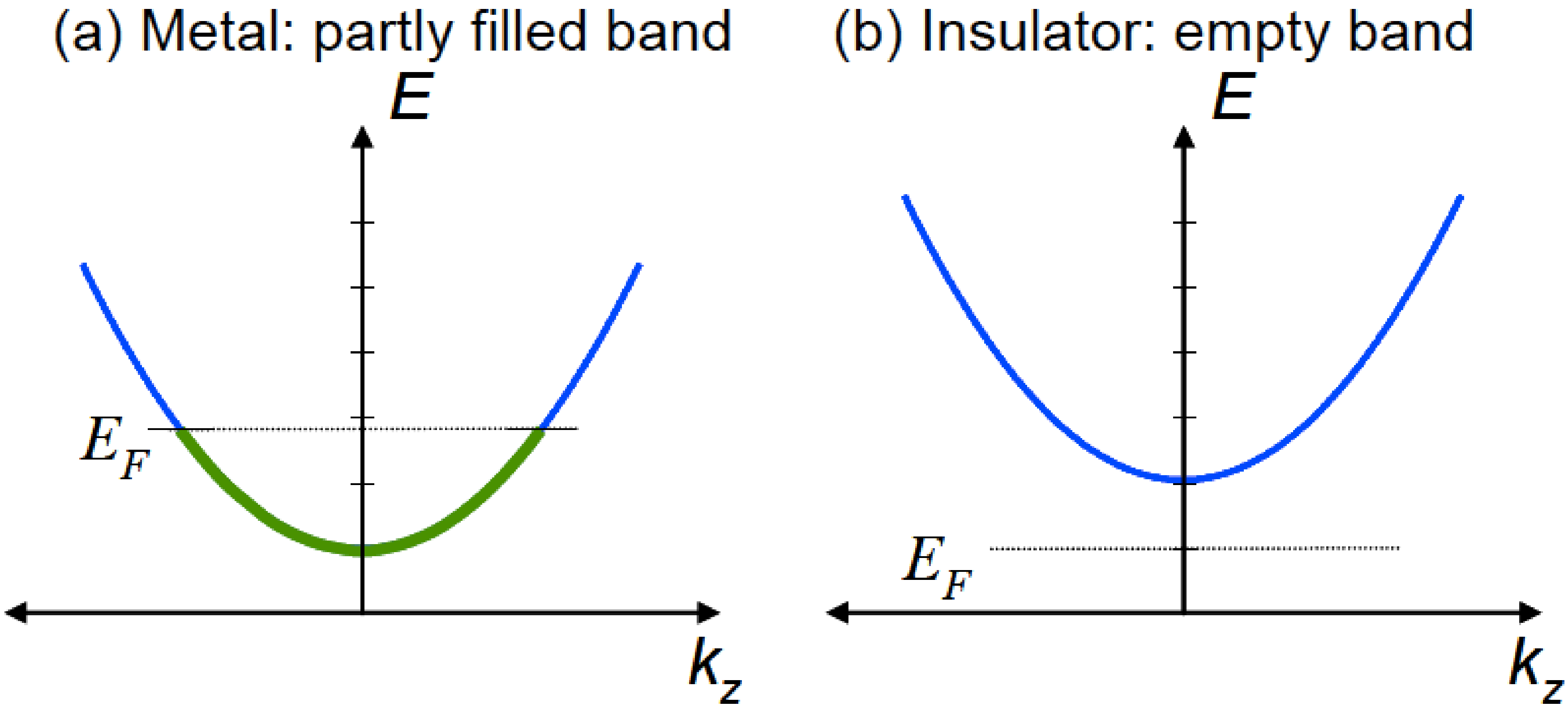
$$E = \frac{\hbar^2}{2m} k^2$$

Current flow



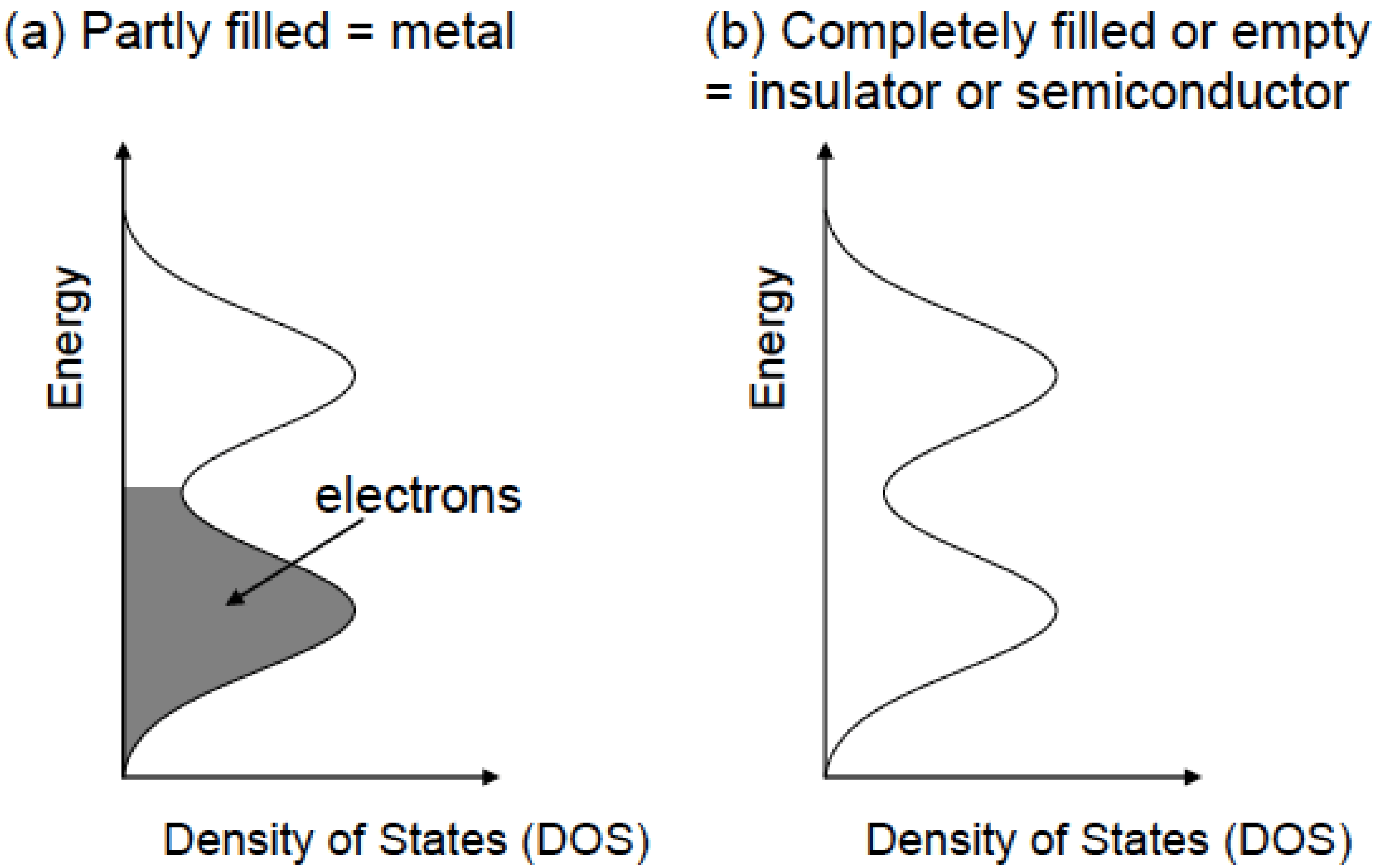
Quasi Fermi levels: *F+* is the energy level when the states with *kz* > 0 are half full,
F- is the corresponding energy level for states with *kz* < 0.

Metal vs Insulator



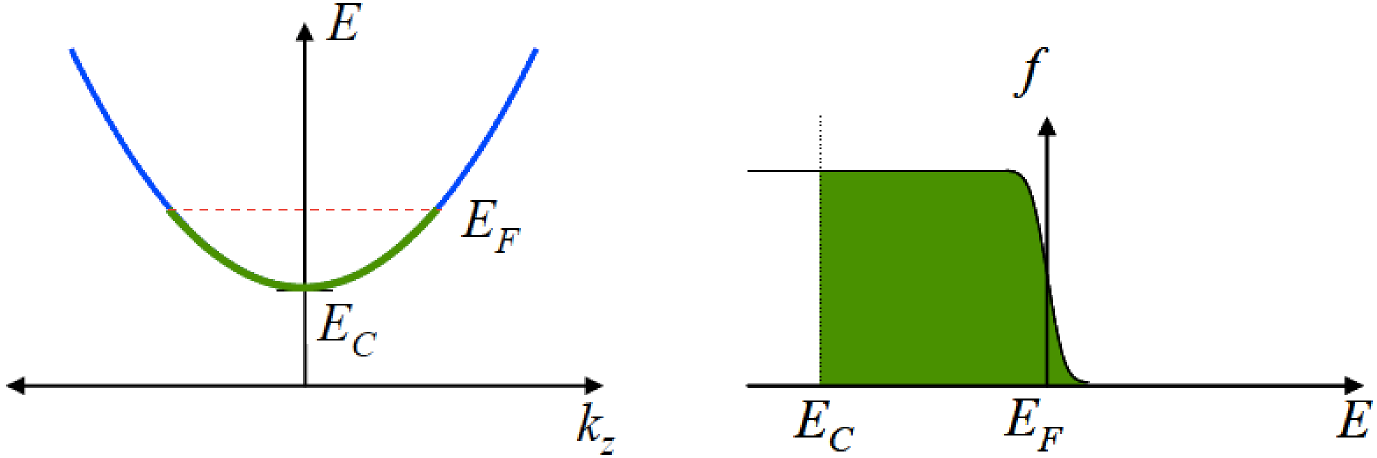
If there are no electrons between *F*+ and *F*-, then the material is an insulator and cannot conduct charge.

Metal vs Insulator



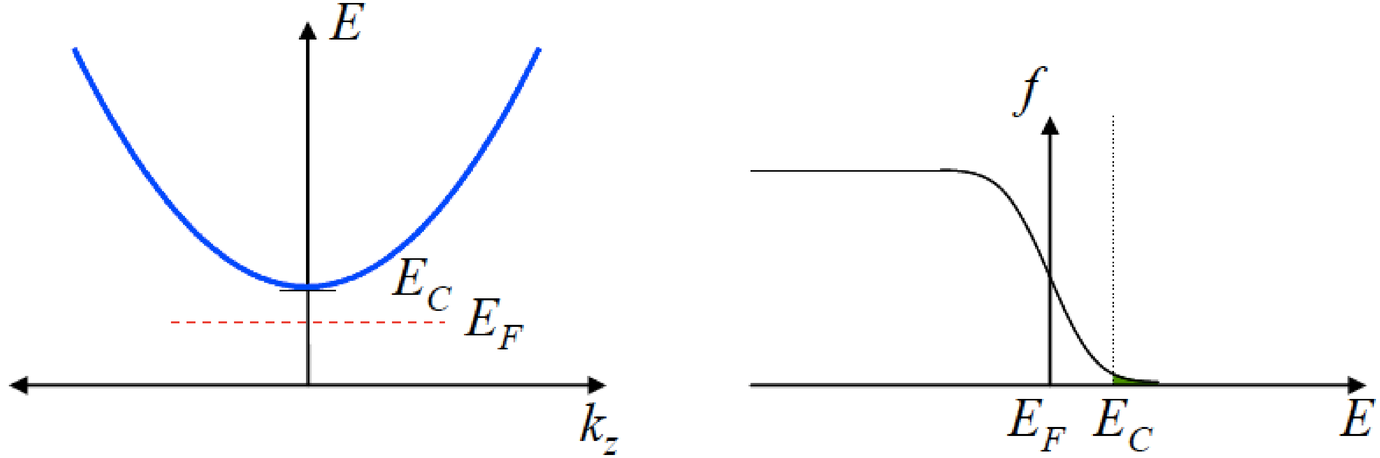
Degenerate case: $E_F - E_C >> k_B T$

(a) Degenerate limit: $f = u(E_F - E)$

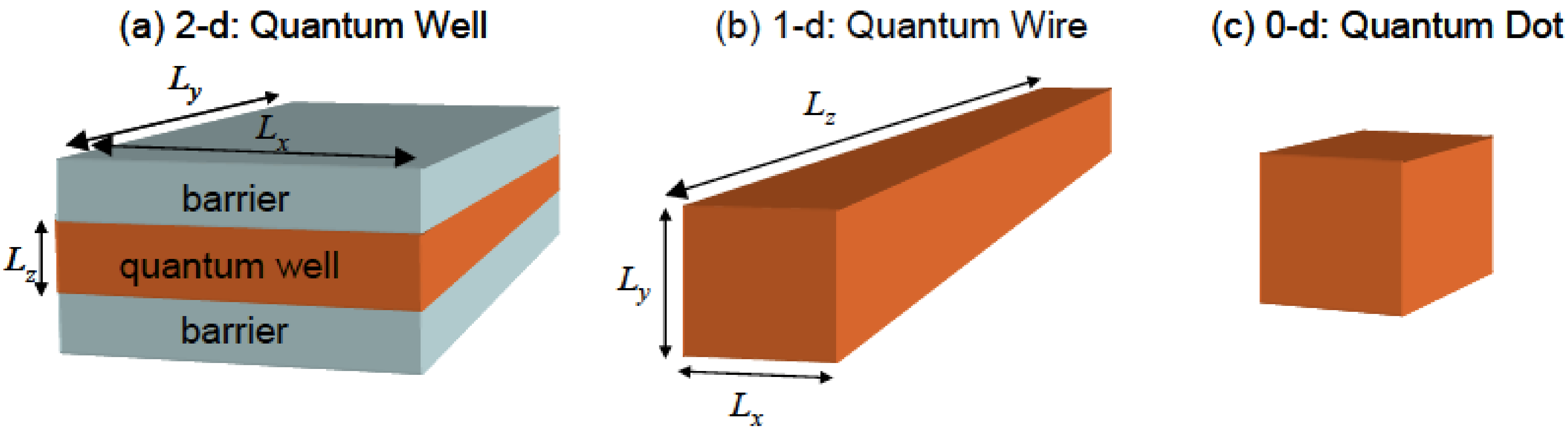


Non-degenerate case: $E_C - E_F >> k_B T$

(b) Non-degenerate limit: $f = \exp[-(E-E_F)/kT]$

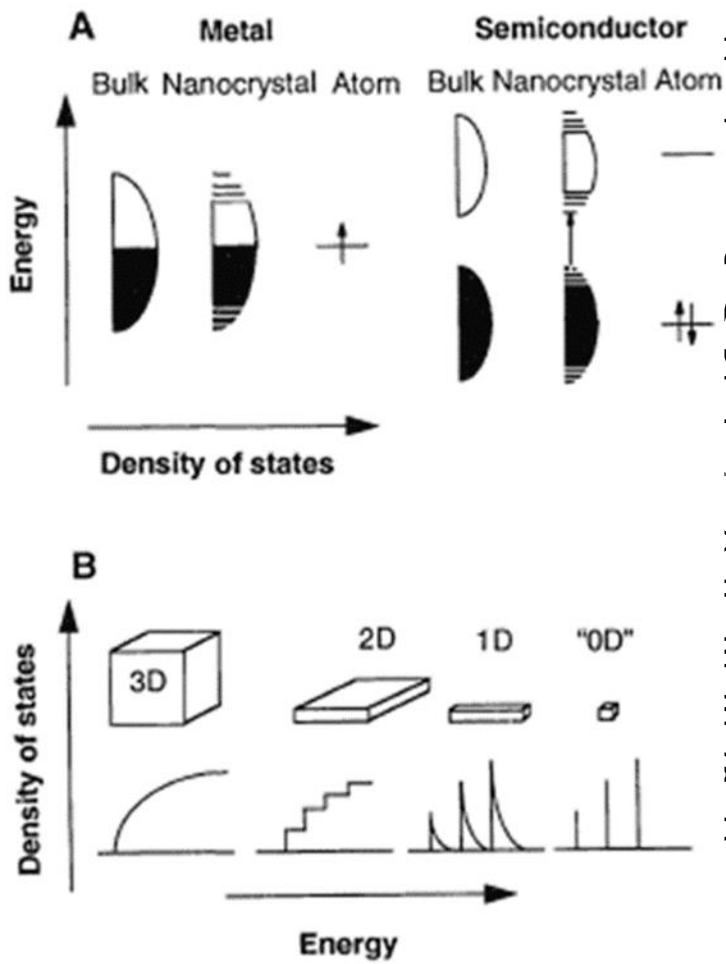


Particle in a "box"



Confinement: the size in a dimension is equal to the electrons wavelength
Un-confined electrons are assumed as plane waves

Bulk material (3D)



e values are allowed. Each point defines a **state**.

The minimum distance in any axis between two states is

$$\Delta k = 2\pi/L$$

olume of the material: $V=L_x L_y L_z$

hat is the volume occupied by one state?

$k^3=\Delta k_x \Delta k_y \Delta k_z=8\pi^3/V$

ow many states do exist in an elementary sphere of
adius dk?

$V(k)/(8\pi^3/V)=4\pi k^2 dk/(8\pi^3/V)$

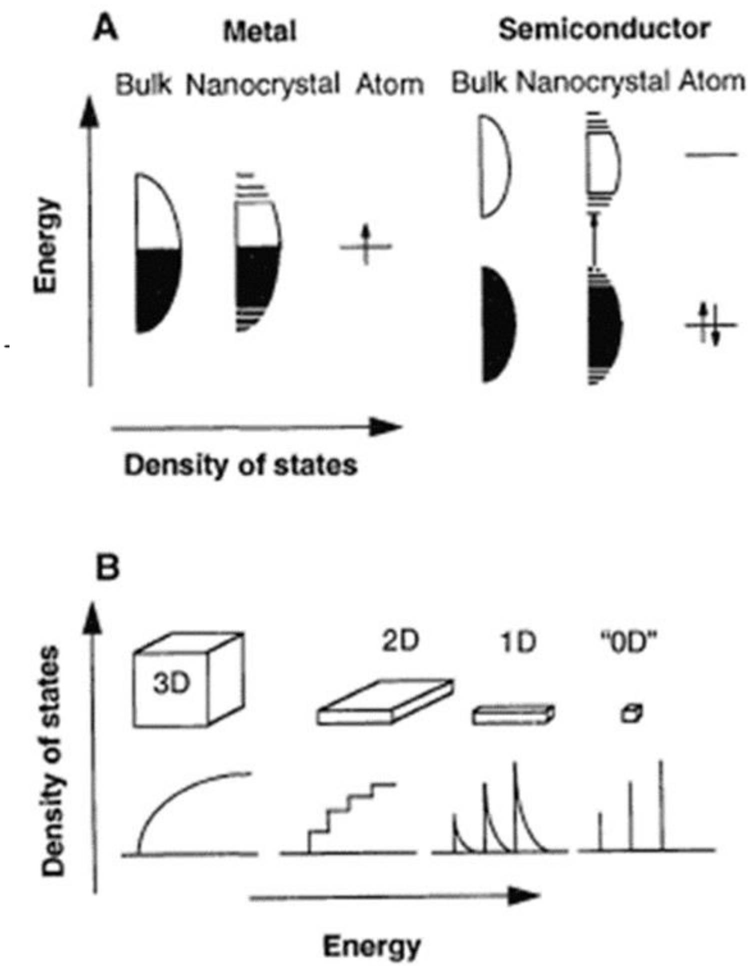
or electrons these states must be multiplied
y 2 (spin-up, spin-down)

ut $E=(h/2\pi)^2k^2/(2m)$ -> $k=(2\pi/h)(2mE)^{1/2}$

o the density of states per per unit of energy
er electron is

$$g(E)dE = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E}dE$$

2D material



minimum distance in any axis between two states is

$\Delta k = 2\pi/L$

of the material: $A = L_x L_y$

t is the area occupied by one state?

$\Delta k_x \Delta k_y = 4\pi^2/A$

many states do exist in an elementary area of

ıs dk?

$)/(4\pi^2/A) = 2\pi k dk/(4\pi^2/A)$

electrons these states must be multiplied

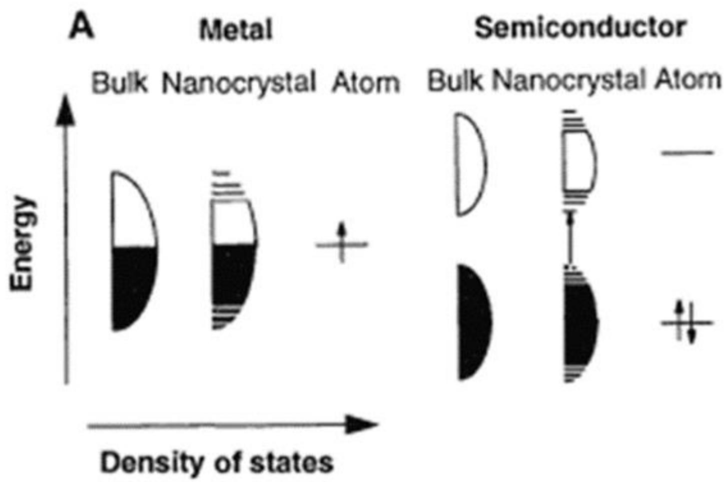
(spin-up, spin-down)

$$= \frac{\hbar^2 \pi^2}{2mL_z^2} n^2 + \frac{\hbar^2 \left(k_x^2 + k_y^2\right)}{2m}, \quad n = 1, 2, \ldots$$

energy $$g(E)dE = \frac{Am}{\pi\hbar^2} \sum_n u(E - E_n) dE$$

per electron is

1D material



minimum distance in any axis between two states is

$\Delta k=2\pi/L$

gth of the material: $L=L_z$

at is the length occupied by one state?

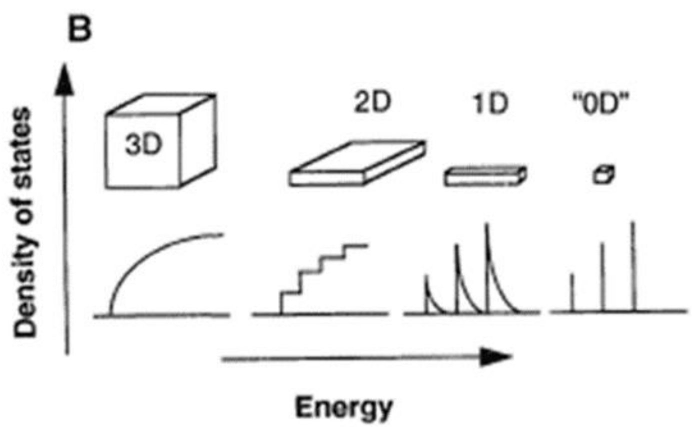
$2\pi/L_z$

many states do exist in an elementary length dk?

$)/(2\pi/L)=dk/(2\pi/L)$

electrons these states must be multiplied

(spin-up, spin-down) and by 2 (left, right)



$$= \frac{\hbar^2\pi^2}{2m}\left(\frac{n_x^2}{L_x^2}+\frac{n_y^2}{L_y^2}\right)+\frac{\hbar^2 k_z^2}{2m}, \quad n_x, n_y = 1, 2, \ldots$$

$$g(E)dE = \frac{2L}{\pi}\sqrt{\frac{m}{2\hbar^2}}\sum_{n_x,n_y}\frac{u\left(E-E_{n_x,n_y}\right)}{\sqrt{E-E_{n_x,n_y}}}dE$$

Energy per electron is

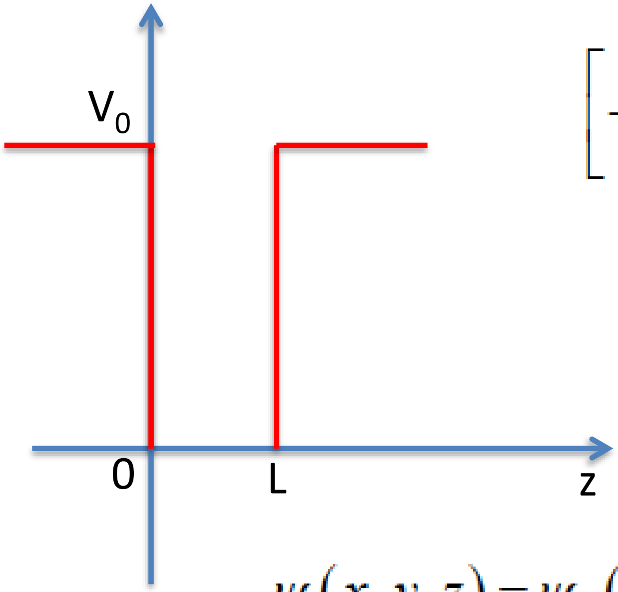
DOS scaling rule

1-d	$\Delta k = \frac{2\pi}{L}$
2-d	$\Delta k^2 = \frac{4\pi^2}{A}$
3-d	$\Delta k^3 = \frac{8\pi^3}{V}$

Potential well

$V_x(x) = 0$
$V_y(y) = 0$
$V_z(z) = V_0\, u(z-L) + V_0\, u(-z)$

u(z)=1 , z<0 else 0.



$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+V_x(x)\right]\psi(x,y,z)+\left[-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}+V_y(y)\right]\psi(x,y,z)$$
$$+\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+V_z(z)\right]\psi(x,y,z)=\left(E_x+E_y+E_z\right)\psi(x,y,z)$$

$$\Psi(x,y,z)=\Psi_x(x)\ \Psi_y(y)\ \Psi_z(z)$$

$$\psi(x,y,z)=\psi_x(x)\psi_y(y)\psi_z(z)=\sqrt{\frac{2}{L}}\sin\left(n\frac{\pi z}{L}\right).\exp\left[ik_x x\right].\exp\left[ik_y y\right]$$

$$E=E_x+E_y+E_z=\frac{\hbar^2 k_x{}^2}{2m}+\frac{\hbar^2 k_y{}^2}{2m}+\frac{n^2\hbar^2\pi^2}{2mL^2}$$

…flash back

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$$

$$\psi(x) = \psi(0)\exp[ikx]$$

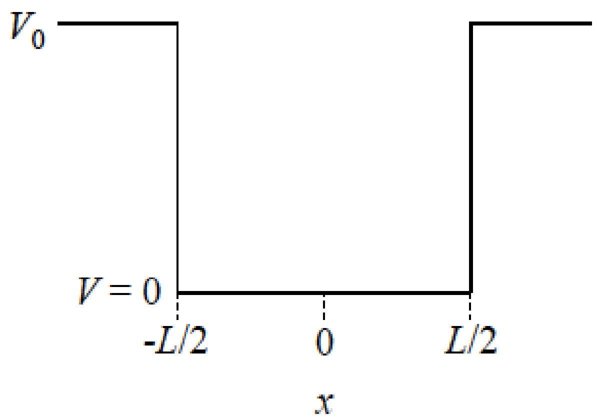
$$k = \sqrt{\frac{2mE}{\hbar^2}}$$

Note

[1] Note that, in general, the form of the second order differential equation that is encountered in this section is $\frac{d^2y}{dx^2} \pm k^2y = 0$. For the (+) sign, the solution is $e^{\pm ikx}$ or $\sin kx$ or $\cos kx$. For the (−) sign, the solution is $e^{\pm kx}$ or $\sinh kx$ or $\cosh kx$. If $y_1(x)$ and $y_2(x)$ represent the two linearly independent solutions, then the general solution is always of the form $y(x) = Ay_1(x) + By_2(x)$, where the constants are chosen to satisfy two boundary conditions. See

Solution in 1D

$V=V_0\neq 0$



x_0=-L/2, L/2

$$\psi_-(x_0)=\psi_+(x_0)$$

$$\frac{d}{dx}\psi_-(x_0)=\frac{d}{dx}\psi_+(x_0)$$

$$\psi(x)=\begin{cases} Ce^{\alpha x} & \text{for } x\leq -L/2 \\ A\cos(kx)+B\sin(kx) & \text{for } -L/2\leq x\leq L/2 \\ De^{-\alpha x} & \text{for } x\geq L/2 \end{cases}$$

$$\alpha=\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

$$k=\sqrt{\frac{2mE}{\hbar^2}},$$

Calculate A, B, C, and D

Infinite Quantum Well

$V_0 \rightarrow \infty$, $a \rightarrow \infty$

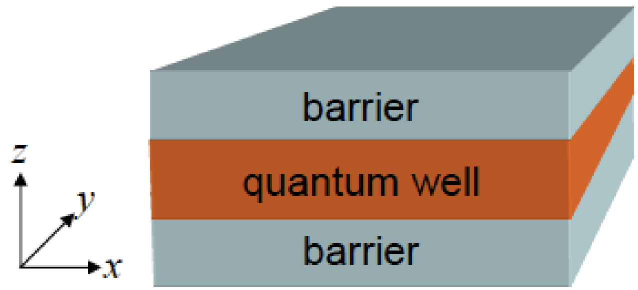
$$\psi(x) = A\sin\left(k\left(x + L/2\right)\right) \qquad \psi=0 \text{ then } kL=n\pi$$

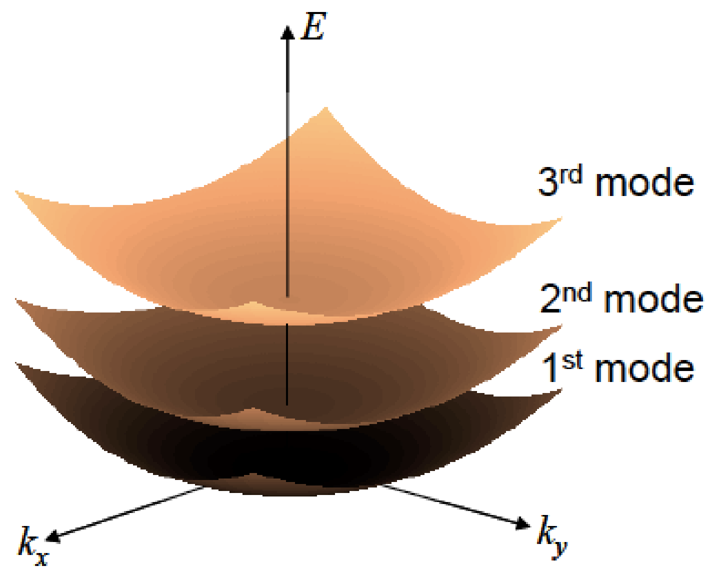
$$\int_{-\infty}^{+\infty} \left|\psi(x)\right|^2 dx = \int_{-L/2}^{L/2} A^2 \cos^2\left(n\pi x/L + n\pi/2\right) dx$$

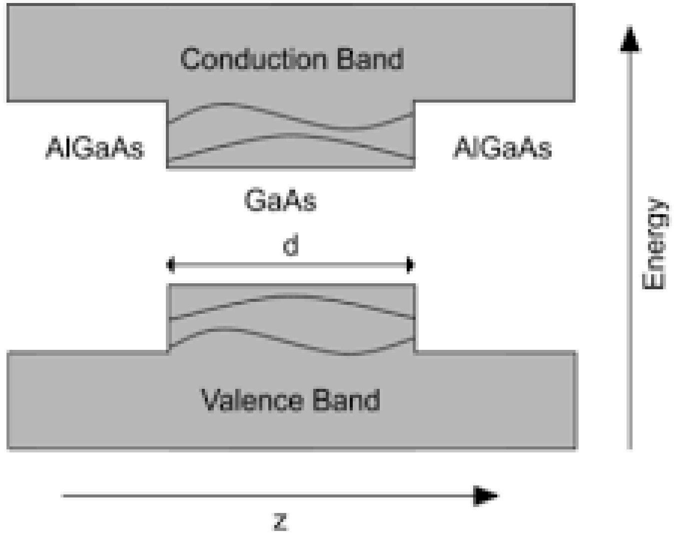
$$A = \sqrt{2/L}$$

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

Potential well







The End

THANK YOU

E-class Support

Lesson	Kassap	Hanson
1		Chap.5
2	3.3	4.1, 4.3,4.4, 4.5.1, Chap.8
3		