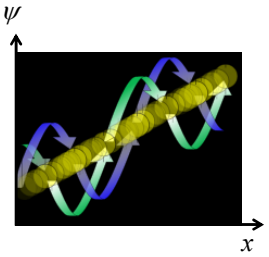
FREE ELECTRON MODEL

Schrodinger Equation

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

Free particle: $V = 0$ ⇒ $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$

$\psi(x) = \psi(0)e^{ikx}$, $\quad k = \sqrt{2mE/\hbar^2}$



Considering the time dependence:

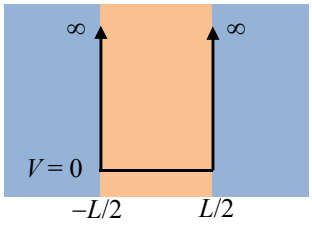
$$\psi(x,t) = \psi(0)e^{i(kx-\omega t)}$$

→ The solution in free space is a plane wave.

Infinite Square Well

$$V_0 \to \infty$$

$$\psi(x) = A \sin kx$$



k is such that $\psi = 0$ at the right boundary:

$$kL = n\pi \qquad k = \frac{n\pi}{L}$$

To normalize the wavefunction and determine A, we integrate:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 \, dx = 1$$

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

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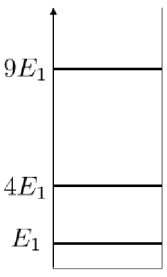
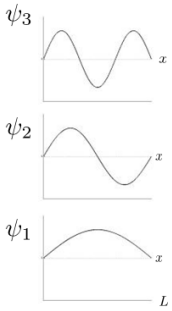
Infinite Square Well

EIGEN ENERGIES



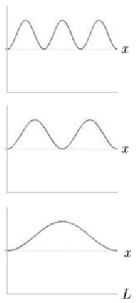
$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \pi^2 n^2}{2mL^2}$$

EIGEN STATES



$$\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi x}{L}$$

PROBABILITY DENSITIES



$$P(x) = |\psi(x)|^2 \, dx$$

- The bound states are quantized – only certain energy levels are allowed.
- The energy levels scale inversely with L^2.

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Ideas & Assumptions

- Valence electrons are assumed to be completely detached from their ions (forming an **electron gas**).
- As in an ideal gas, electron-electron interactions are completely neglected. The electrostatic fields in metals are weak because of the screening effect.
- The crystal lattice is not explicitly taken into account. A quantum-mechanical justification is given by Bloch's Theorem: An unbound electron moves in a periodic potential as a free electron in vacuum, except for the electron mass m becoming an effective mass m^* which may deviate considerably from m.
- According to the Pauli exclusion principle, each phase space element $(\Delta k)^3(\Delta x)^3$ can be occupied only by two electrons (one per spin).

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3-D Schrodinger Equation

- Kinetic energy operator: $\hat{T} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m} = -\frac{\hbar^2}{2m}\left(\frac{d^2}{dx^2} + \frac{d^2}{dx^2} + \frac{d^2}{dx^2}\right)$
- Potential energy operator: $\hat{V} = V_x(x) + V_y(y) + V_z(z)$
- Wavefunction: $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$
- Electron energy: $E = E_x + E_y + E_z$

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

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Bulk Material

$$V(x,y,z) = V_x(x) + V_y(y) + V_z(z)$$

- A bulk material potential:

$$V_x(x) = 0$$
$$V_y(y) = 0$$
$$V_z(z) = 0$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x,y,z) - \frac{\hbar^2}{2m}\frac{d^2}{dy^2}\psi(x,y,z)$$
$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\psi(x,y,z) = (E_x + E_y + E_z)\psi(x,y,z)$$

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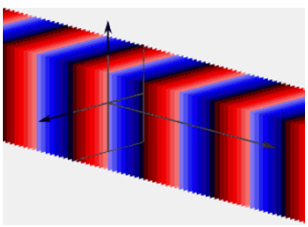
Solution

- Wavefunctions: $\psi(x,y,z) = \psi_x(x)\psi_y(y)\psi_z(z)$
$= \psi_0 e^{ik_x x} e^{ik_y y} e^{ik_z z}$

- Energies: $E = E_x + E_y + E_z = \frac{\hbar^2 k_x^2}{2m} + \frac{\hbar^2 k_y^2}{2m} + \frac{\hbar^2 k_z^2}{2m}$



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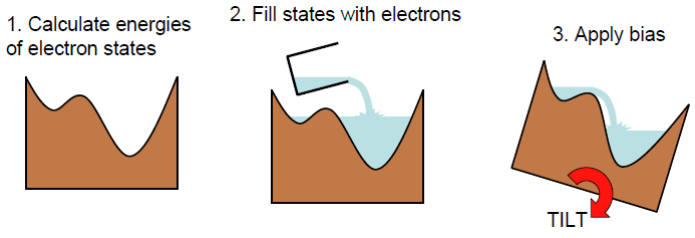
Filling-Up States

- We will learn the principles of electron statistics and how to fill the states with electrons.
- Our goal is to apply voltage to set electrons in motion.



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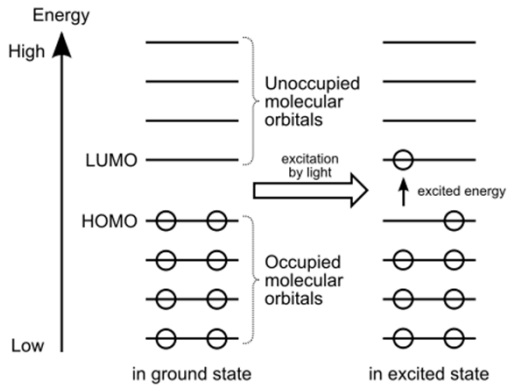
Number of Electrons

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

$g(E)$: density of states



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How Many Electrons?

- The Pauli exclusion principle forbids multiple identical electrons from occupying the same state simultaneously.
- Do not forget about spin → +1/2 or –1/2, spin up or spin down.
- If we were to add electrons to an otherwise *empty* material, and then left the electrons alone, they would ultimately occupy their *equilibrium* distribution.
- At equilibrium, electrons have the same material temperature and the lowest energy states are filled first.

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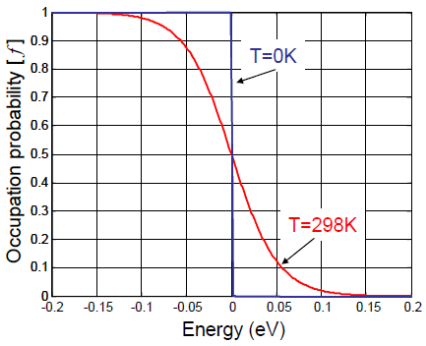
Fermi-Dirac Statistics

- Fermi-Dirac Statistics: $f(E,\mu)=\dfrac{1}{1+e^{(E-\mu)/k_bT}}$
- At $T=0$ K: $f(E-\mu)=u(\mu-E)$



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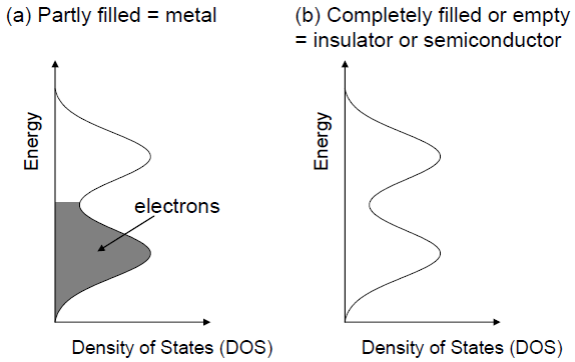
Density of States

- To determine whether a material is a metal or an insulator, and to calculate the magnitude of the current under applied bias, we need the density of states (DOS).
- **DOS:** Number of states per unit energy.



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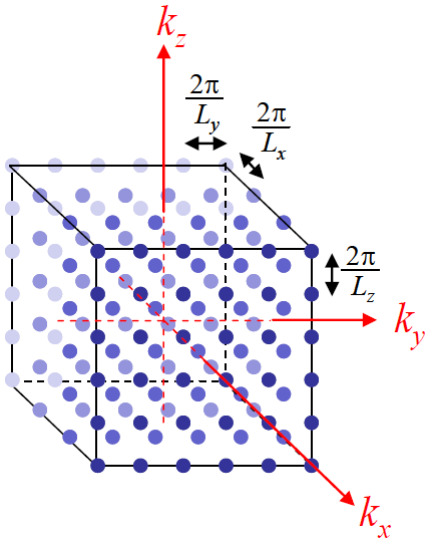
Density of States

- Allowed k_x, k_y, and k_z depend on boundary conditions.
- The volume of k-space per allowed state:

$$\Delta k^3 = \Delta k_x \Delta k_y \Delta k_z = \frac{2\pi}{L_x}\frac{2\pi}{L_y}\frac{2\pi}{L_z} = \frac{8\pi^3}{V}$$



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Density of States

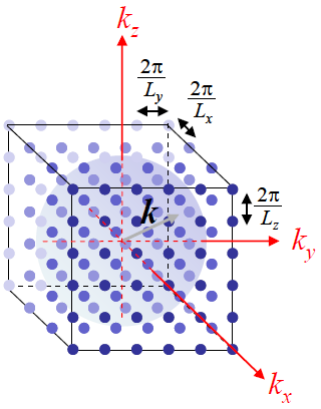
- The number of modes within a spherical shell of thickness *dk*:

$$g(k)\,dk = 2\times\frac{1}{8\pi^3/V}\times 4\pi k^2 dk$$

- Substituting *k* by *E*:

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

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



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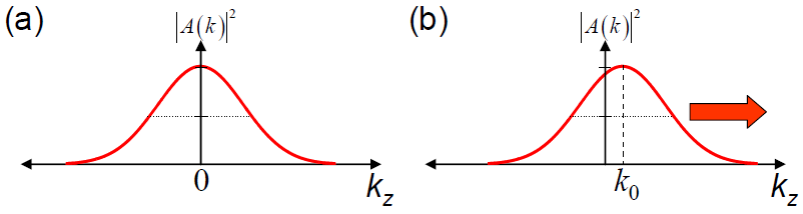
Current

- What is the current if we have a Gaussian wavepacket for moving electrons?



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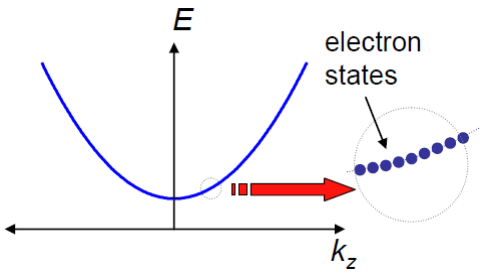
Electron States

- Electrons in a wire occupy states with different energies and wavenumbers.



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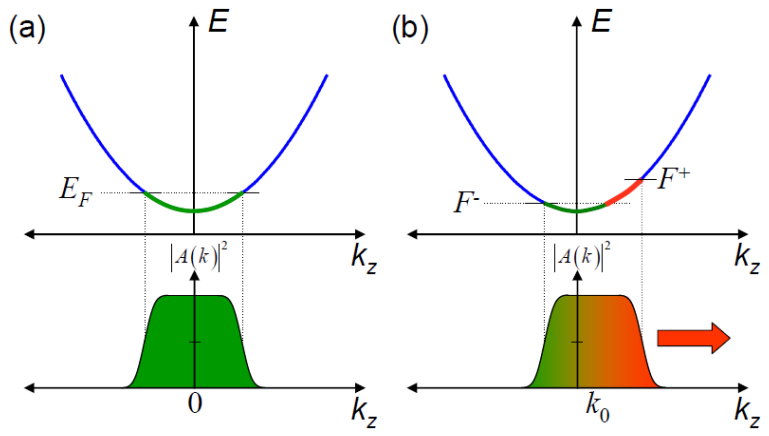
Current

a) $+k_z$ and $-k_z$ states are filled equally. There is no net current.

b) $+k_z$ and $-k_z$ states are not filled equally. There is net current.



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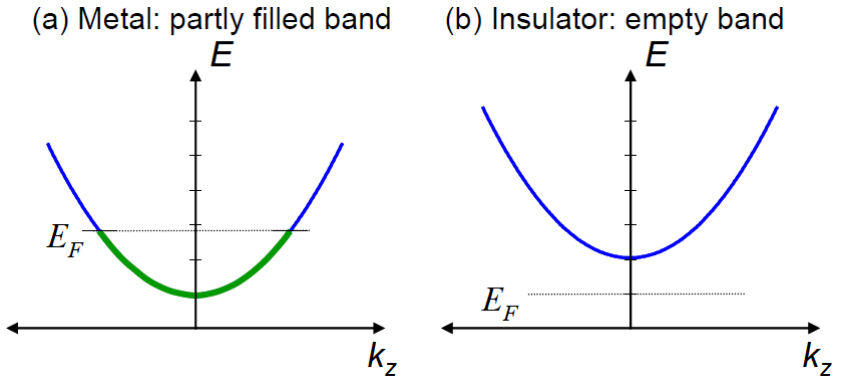
Metals and Insulators

- **Metals:** Electrons between F^+ and F^-.
- **Insulators:** No electron between F^+ and F^-.



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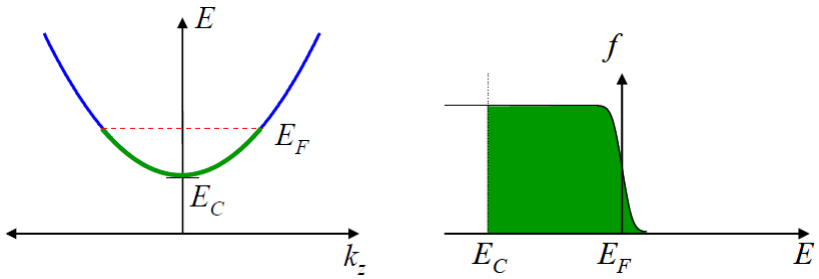
Degenerate Limit

$$E_F - E_C \gg k_b T$$

- The distribution function is modeled by a unit step:

$$f(E) = u(E_F - E)$$



- **Thermal blurring of electron distribution is insignificant!**

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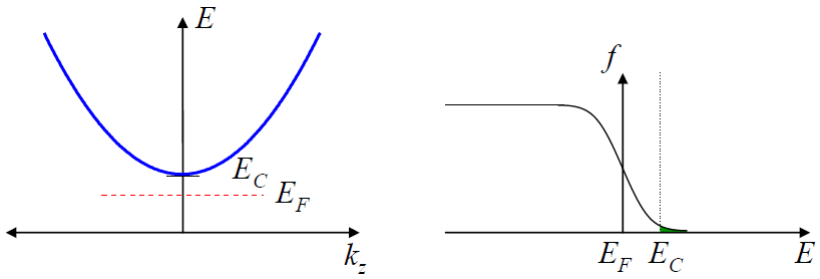
Non-Degenerate Limit

$$E_C - E_F \gg k_b T$$

- The distribution function is modeled by a unit step:

$$f(E) = e^{-(E-E_F)/k_b T}$$



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