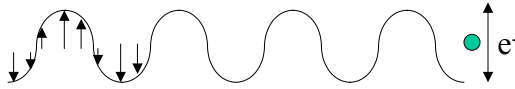


Response of Free e- to AC Electric Fields

- Microscopic picture



$$E_z = E_0 e^{-i\omega t}$$

$B=0$ in conductor,

and $\vec{F}(\vec{E}) \gg \vec{F}(\vec{B})$

$$\frac{dp(t)}{dt} = -\frac{p(t)}{\tau} - eE_0 e^{-i\omega t}$$

try $p(t) = p_0 e^{-i\omega t}$

$$-i\omega p_0 = -\frac{p_0}{\tau} - eE_0$$

$$p_0 = \frac{eE_0}{i\omega - \frac{1}{\tau}}$$

$\omega \gg 1/\tau$, p out of phase with E

$$p_0 = \frac{eE_0}{i\omega} \quad \omega \rightarrow \infty, p \rightarrow 0$$

$\omega \ll 1/\tau$, p in phase with E

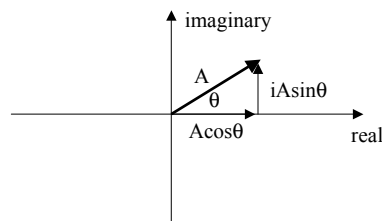
$$p_0 = eE_0 \tau$$



Complex Representation of Waves

$\sin(kx - \omega t)$, $\cos(kx - \omega t)$, and $e^{-i(kx - \omega t)}$ are all waves

$e^{-i(kx - \omega t)}$ is the complex one and is the most general

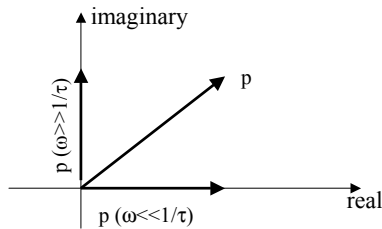


$$e^{i\theta} = \cos\theta + i\sin\theta$$



Response of e- to AC Electric Fields

- Momentum represented in the complex plane



Instead of a complex momentum, we can go back to macroscopic and create a complex J and σ

$$J(t) = J_0 e^{-i\omega t} \quad J_0 = -nev = \frac{-nep_0}{m} = \frac{ne^2}{m(\frac{1}{\tau} - i\omega)} E_0$$

$$\sigma = \frac{\sigma_0}{1 - i\omega\tau}, \sigma_0 = \frac{ne^2\tau}{m}$$

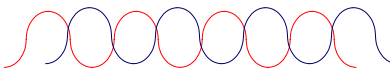
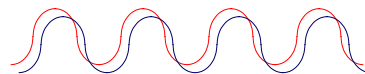


3.225

© E.A. Fitzgerald-1999 3

Response of e- to AC Electric Fields

- Low frequency ($\omega \ll 1/\tau$)
 - electron has many collisions before direction change
 - Ohm's Law: J follows E, σ real
- High frequency ($\omega \gg 1/\tau$)
 - electron has nearly 1 collision or less when direction is changed
 - J imaginary and 90 degrees out of phase with E, σ is imaginary



Qualitatively:

$\omega\tau \ll 1$, electrons in phase, re-irradiate, $E_i = E_r + E_t$, reflection

$\omega\tau \gg 1$, electrons out of phase, electrons too slow, less interaction, transmission $\epsilon = \epsilon_r \epsilon_0$, $\epsilon_r = 1$

$$\tau \approx 10^{-14} \text{ sec}, v\lambda = c, v = \frac{3 \times 10^{10} \text{ cm/sec}}{5000 \times 10^{-8} \text{ cm}} \approx 10^{14} \text{ Hz}$$

E-fields with frequencies greater than visible light frequency expected to be beyond influence of free electrons



3.225

© E.A. Fitzgerald-1999 4

Response of Light to Interaction with Material

- Need Maxwell's equations
 - from experiments: Gauss, Faraday, Ampere's laws
 - second term in Ampere's is from the unification
 - electromagnetic waves!

SI Units (MKS)

$$\begin{aligned} \nabla \cdot \vec{D} &= \rho \\ \nabla \cdot \vec{B} &= 0 \\ \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{H} &= \vec{J} + \frac{\partial \vec{D}}{\partial t} \\ \vec{D} &= \epsilon_0 \vec{E} + \vec{P} = \epsilon \vec{E} \\ \vec{B} &= \mu_0 \vec{H} + \mu_0 \vec{M} = \mu \vec{H} \\ \mu &= \mu_r \mu_0; \epsilon = \epsilon_r \epsilon_0 \end{aligned}$$

Gaussian Units (CGS)

$$\begin{aligned} \nabla \cdot \vec{D} &= 4\pi\rho \\ \nabla \cdot \vec{B} &= 0 \\ \nabla \times \vec{E} &= -\frac{1}{c} \frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{H} &= \frac{4\pi}{c} \vec{J} + \frac{1}{c} \frac{\partial \vec{D}}{\partial t} \\ \vec{D} &= \vec{E} + 4\pi\vec{P} \\ \vec{B} &= \vec{H} + 4\pi\vec{M} \end{aligned}$$



Waves in Materials

- Non-magnetic material, $\mu = \mu_0$
- Polarization non-existent or swamped by free electrons, $P=0$

$$\begin{aligned} \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} \\ \nabla \times \vec{B} &= \mu_0 \vec{J} + \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} \\ \nabla \times (\nabla \times \vec{E}) &= -\frac{\partial \nabla \times \vec{B}}{\partial t} \\ -\nabla^2 \vec{E} &= -\frac{\partial}{\partial t} [\mu_0 \vec{J} + \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t}] \\ \nabla^2 \vec{E} &= \mu_0 \sigma \frac{\partial \vec{E}}{\partial t} + \mu_0 \epsilon_0 \frac{\partial^2 \vec{E}}{\partial t^2} \end{aligned}$$

For a typical wave,

$$E = E_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \omega t)} = E_0 e^{i\mathbf{k} \cdot \mathbf{r}} e^{-i\omega t} = E(\mathbf{r}) e^{-i\omega t}$$

$$\nabla^2 E(\mathbf{r}) = -i\omega \mu_0 \sigma E(\mathbf{r}) - \mu_0 \epsilon_0 \omega^2 E(\mathbf{r})$$

$$\nabla^2 E(\mathbf{r}) = -\frac{\omega^2}{c^2} \epsilon(\omega) E(\mathbf{r}) \quad \text{Wave Equation}$$

$$\epsilon(\omega) = 1 + \frac{i\sigma}{\epsilon_0 \omega}$$

$$E(\mathbf{r}) = E_0 e^{i\mathbf{k} \cdot \mathbf{r}}$$

$$k^2 = \frac{\omega^2}{c^2} \epsilon(\omega)$$

$$v = \frac{\omega}{k} = \frac{c}{\sqrt{\epsilon(\omega)}}$$



Waves in Materials

- Waves slow down in materials (depends on $\epsilon(\omega)$)
- Wavelength decreases (depends on $\epsilon(\omega)$)
- Frequency dependence in $\epsilon(\omega)$

$$\epsilon(\omega) = 1 + \frac{i\sigma}{\epsilon_0\omega} = 1 + \frac{i\sigma_0}{\epsilon_0\omega(1-i\omega\tau)}$$

$$\epsilon(\omega) = 1 + \frac{i\omega_p^2\tau}{\omega - i\omega^2\tau}$$

$$\omega_p^2 = \frac{ne^2}{\epsilon_0 m} \quad \text{Plasma Frequency}$$

For $\omega\tau \gg 1$, $\epsilon(\omega)$ goes to 1

For an excellent conductor (σ large), ignore 1, look at case for $\omega\tau \ll 1$

$$\epsilon(\omega) \approx \frac{i\omega_p^2\tau}{\omega - i\omega^2\tau} \approx \frac{i\omega_p^2\tau}{\omega}$$



Waves in Materials

$$k = \frac{\omega}{c} \sqrt{\epsilon(\omega)} = \frac{\omega}{c} \sqrt{i} \sqrt{\frac{\sigma_0}{\omega\epsilon_0}}$$

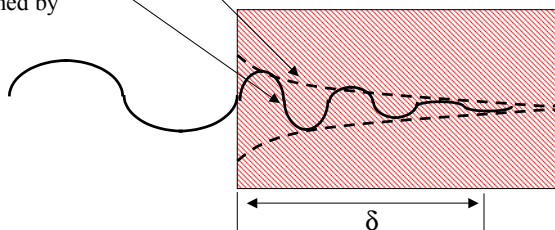
$$k = \frac{\omega}{c} \left(\frac{1+i}{\sqrt{2}} \right) \sqrt{\frac{\sigma_0}{\omega\epsilon_0}} = \left(\sqrt{\frac{\sigma_0\omega}{2\epsilon_0 c^2}} + i \sqrt{\frac{\sigma_0\omega}{2\epsilon_0 c^2}} \right)$$

For a wave $E = E_0 e^{i(kz - \omega t)}$ Let $k = k_{\text{real}} + k_{\text{imaginary}} = k_r + ik_i$

$$E = E_0 e^{i[k_r z - \omega t]} e^{-|k_i|z}$$

The skin depth can be defined by

$$\delta = \frac{1}{|k_i|} = \sqrt{\frac{2\epsilon_0 c^2}{\sigma\omega}} = \sqrt{\frac{2}{\sigma\mu_0\omega}}$$



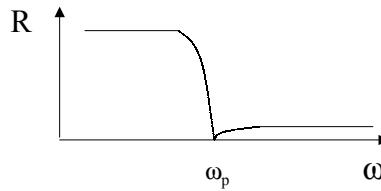
Waves in Materials

For a material with any σ_p , look at case for $\omega\tau \gg 1$

$$\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2}$$

$\omega < \omega_p$, ϵ is negative, $k=k_i$, wave reflected

$\omega > \omega_p$, ϵ is positive, $k=k_r$, wave propagates



Success and Failure of Free e- Picture

- Success

- Metal conductivity
- Hall effect valence=1
- Skin Depth
- Wiedmann-Franz law

$K/\sigma = \text{thermal conduct./electrical conduct.} \sim CT$

$$K = \frac{1}{3} c_v v_{therm}^2 \tau$$

$$c_v = \left(\frac{\partial E}{\partial T} \right)_v = \frac{3}{2} n k_b ; v_{therm}^2 = \frac{3 k_b T}{m}$$

$$K = \frac{1}{3} \left(\frac{3}{2} n k_b \right) \left(\frac{3 k_b T}{m} \right) \tau = \frac{3}{2} \frac{n k_b^2 T \tau}{m}$$

- Examples of Failure

- Insulators, Semiconductors
- Hall effect valence > 1
- Thermoelectric effect
- Colors of metals

$$\sigma = \frac{n e^2 \tau}{m}$$

Therefore : $\frac{K}{\sigma} = \frac{3}{2} \left(\frac{k_b}{e} \right)^2 T$
 $\sim C!$

Luck: $c_{vreal} = c_{vclass} / 100;$
 $v_{real}^2 = v_{class}^2 * 10$

0



Wiedmann-Franz 'Success'

EXPERIMENTAL THERMAL CONDUCTIVITIES AND LORENZ NUMBERS OF SELECTED METALS

ELEMENT	273 K		373 K	
	κ (watt-cm-K)	$\kappa/\sigma T$ (watt-ohm-K ²)	κ (watt-cm-K)	$\kappa/\sigma T$ (watt-ohm-K ²)
Li	0.71	2.22×10^{-7}	0.73	2.43×10^{-7}
Na	1.38	2.12		
K	1.0	2.23		
Rb	0.6	2.42		
Cu	3.85	2.20	3.82	2.29
Ag	4.18	2.31	4.17	2.38
Au	3.1	2.32	3.1	2.36
Hg	2.3	2.36	1.7	2.42
Mg	1.5	2.14	1.5	2.25
Nb	0.52	2.90	0.54	2.78
Zn	0.80	2.61	0.73	2.88
Zr	1.13	2.28	1.1	2.30
Cd	1.0	2.49	1.0	
Al	2.38	2.14	2.30	2.19
Ir	0.88	2.58	0.80	2.60
Tl	0.5	2.75	0.45	2.75
Sn	0.64	2.48	0.60	2.54
Pb	0.38	2.64	0.35	2.53
Bi	0.09	3.53	0.08	3.35
Sb	0.18	2.57	0.17	2.69

Thermoelectric Effect

Exposed Failure when c_v and v^2 are not both in property

$$E = QVT$$

$$\text{Thermopower } Q \text{ is } Q = -\frac{c_v}{3ne} = -\frac{\frac{3}{2}nk_b}{3ne} = -\frac{nk_b}{2e}$$

Thermopower is about 100 times too large!



3.225

© E.A. Fitzgerald-1999 11

Waves in Vacuum

- $J, \rho = 0$
- $\mu = \mu_0; \epsilon = \epsilon_0$

$$\nabla^2 E = \mu_0 \epsilon_0 \frac{\partial^2 E}{\partial t^2}$$

Wave Equation

For typical wave:

$$E = E_0 e^{ik \cdot r - \omega t} \quad k = 2\pi/\lambda; \omega = 2\pi\nu$$

$$k^2 = \mu_0 \epsilon_0 \omega^2$$

$$\Rightarrow \omega/k = \nu\lambda = (\mu_0 \epsilon_0)^{-1/2}$$

For constant phase: $(kx - \omega t)$

$$v_{\text{phase}} = \omega/k = c \rightarrow c = (\mu_0 \epsilon_0)^{-1/2}$$

Example:
Violet light ($\nu = 7.5 \times 10^{14}$ Hz)
 $\lambda = c/\nu = 400$ nm
 $k = 2\pi/\lambda = 1.57 \times 10^7 \text{ m}^{-1}$
 $\omega = 2\pi\nu = 4.71 \times 10^{15} \text{ s}^{-1}$



3.225

After Livingston

12

Waves in Materials; Skin Depth

$$\nabla^2 E = \mu\epsilon \frac{\partial^2 E}{\partial t^2} + \mu\sigma \frac{\partial E}{\partial t} \quad ; \mu \cong \mu_0$$

$$k^2 = \omega^2 \mu\epsilon + i\omega\mu\sigma$$

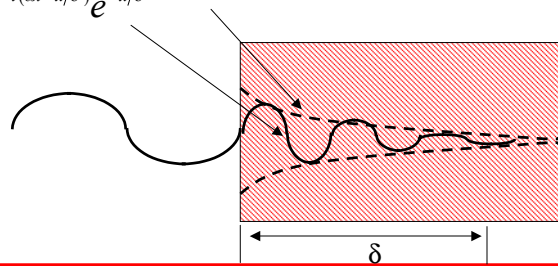
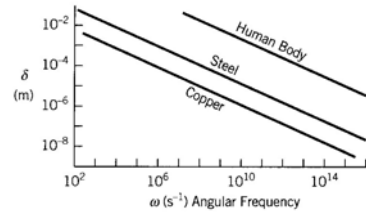
$$k \approx (i\omega\mu\sigma)^{1/2} \quad \text{Conductive materials}$$

$$= \pm \frac{1+i}{\sqrt{2}} (\omega\mu\sigma)^{1/2} = \pm \frac{1+i}{\delta}$$

$$\Rightarrow E = E_0 e^{i(kx - \omega t)} = E_0 e^{-i(\omega t - x/\delta)} e^{-x/\delta}$$

The skin depth is defined by

$$\delta = \left(\frac{2}{\omega\mu\sigma} \right)^{1/2}$$



3.225

After Livingston

13

Plasma Frequency

Remember: $k^2 = \omega^2 \mu\epsilon + i\omega\mu\sigma$

where $\sigma = \frac{\sigma_0}{1 - i\omega\tau} \approx \frac{-\sigma_0}{i\omega\tau} \quad (\omega\tau \gg 1)$

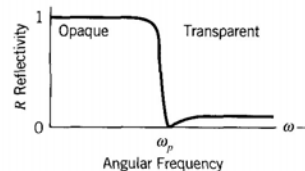
then $k^2 \cong \omega^2 \mu\epsilon - \frac{\mu\sigma_0}{\tau} = \omega^2 \mu\epsilon \left(1 - \frac{\omega_p^2}{\omega^2} \right)$

where $\omega_p \cong \left(\frac{ne^2}{m\epsilon} \right)^{1/2} \Rightarrow$ Plasma Frequency

\Rightarrow For $\omega > \omega_p$; k is real number no attenuation!
 $\omega < \omega_p$; k contains imaginary component, wave reflected

\Rightarrow Criteria for transparent electrode?

(Example: $n = 5.8 \times 10^{27} \text{ m}^{-3}$; $\omega_p = 4.3 \times 10^{15} \text{ s}^{-1}$)



3.225

After Livingston

14

Wave-particle Duality: Electrons are not *just* particles

- Compton, Planck, Einstein
 - light (xrays) can be ‘particle-like’
- DeBroglie
 - matter can act like it has a ‘wave-nature’
- Schrodinger, Born
 - Unification of wave-particle duality, Schrodinger Equation



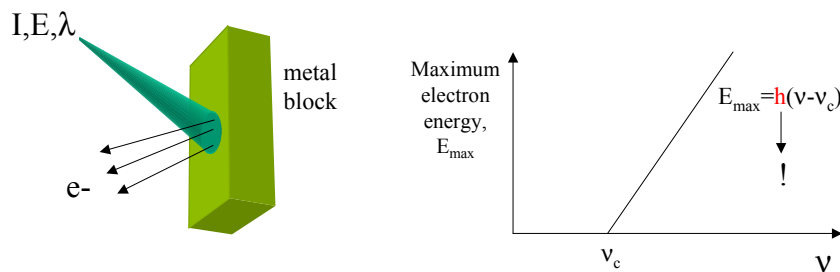
3.225

© E. Fitzgerald-1999

15

Light is always quantized: Photoelectric effect (Einstein)

- Photoelectric effect shows that $E=hf$ even outside the box



For light with $\nu < \nu_c$, no matter what the intensity, no e^-



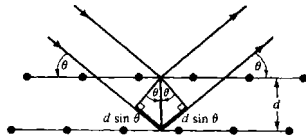
3.225

© E. Fitzgerald-1999

16

DeBroglie: Matter is Wave

- His PhD thesis!
- $\lambda = h/p$ also for matter
- To verify, need very light matter (p small) so λ is large enough
- Need small periodic structure on scale of λ to see if wave is there (diffraction)
- Solution: electron diffraction from a crystal



$$N\lambda = 2d \sin \theta$$

For small θ , $\theta \sim \lambda/d$, so λ must be on order of d in order to measure easily



Unification: Wave-particle Duality

Ψ must be able to represent everything from a particle to a wave (the two extremes)

wave

$$\Psi = A e^{i(kx - \omega t)}$$



k and p known exactly

particle

$$\Psi = \sum_n a_n e^{i(k_n x - \omega_n t)}$$



$n = \infty$ to create a delta function in Ψ^2

generalized

$$\Psi = \sum_n a_n e^{i(k_n x - \omega_n t)}$$



Quantum Mechanics - Wave Equation



Classical Hamiltonian

$$\frac{p^2}{2m} + V(x, y, z) = E$$

QM Operators

$$p = \left(\frac{\hbar}{i}\right)\Delta \quad E = -\left(\frac{\hbar}{i}\right)\frac{\partial}{\partial t}$$

$$\boxed{-\frac{\hbar^2}{2m}\Delta^2\psi + V(x, y, z)\psi = -\frac{\hbar}{i}\frac{\partial\psi}{\partial t}}$$

1. ψ and $\Delta\psi$ must be finite, continuous and single valued.
2. $\psi\psi^*$ real with $\psi\psi^*dV$ = probability of finding particle in volume dV .
3. Average or expectation value of variable

$$\langle\alpha\rangle = \int_V \psi^* \alpha_{op} \psi dV$$



Time and Spatial Dependence of ψ



Assume $\psi(x, y, z, t)$ separable into $\psi(x, y, z)$ and $\phi(t)$

Applying separation of variables:

$$\frac{-\hbar^2}{2m} \frac{\nabla^2\psi}{\psi} + V = -\frac{\hbar}{i} \frac{1}{\phi} \frac{\partial\phi}{\partial t} = \varepsilon = \text{constant}$$

Time-Dependent Equation:

$$\phi(t) = Ae^{-i(\varepsilon/\hbar)t} = Ae^{-i\omega t}$$

$$\Rightarrow \boxed{\varepsilon = \hbar\omega}$$

Time-Independent Equation:

$$\nabla^2\psi + \frac{2m}{\hbar^2}(\varepsilon - V)\psi = 0$$

Solutions: ψ_n -eigenfunctions; ε_n -eigenvalues



Free Particle

- One dimensional $V = 0$

$$\frac{d^2\psi}{dx^2} = -\frac{2m\varepsilon}{\hbar^2}\psi = -k^2\psi$$

$$\psi = Ae^{ikx}$$

$$\boxed{\varepsilon = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}}$$

$$\boxed{p = \hbar k} \quad \text{Crystal Momentum}$$

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

- Momentum

$$\langle p_x \rangle = \int \psi^* \frac{\hbar}{i} \frac{\partial \psi}{\partial x} dx = \hbar k$$



3.225

© H.L. Tuller-2001

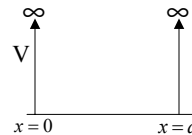
21

Particle in Box

$$\psi = Ae^{ikx} + Be^{-ikx}; k^2 = \frac{2m\varepsilon}{\hbar^2}$$

Boundary Conditions:

- $\psi(0) = \psi(d) = 0$
- $\psi(0) = A + B = 0 \quad \Rightarrow A = -B$
- $\psi(d) = A(e^{ikd} - e^{-ikd}) = 0 \quad \Rightarrow 2A \sin kd = 0$



$$\boxed{k = \frac{n\pi}{d} \quad n = 1, 2, 3, \dots}$$

$$\boxed{\psi = \sqrt{\frac{2}{d}} \sin\left(\frac{n\pi x}{d}\right) \quad n = 1, 2, 3, \dots}$$



3.225

© H.L. Tuller-2001

22

Particle in Box



$$\Psi_n(x, y, z) = A \sin k_1 x \cdot \sin k_2 y \cdot \sin k_3 z$$

$$k^2 = k_1^2 + k_2^2 + k_3^2 \quad k_i = \frac{n_i \pi}{d}; \quad n_i = 1, 2, 3 \dots$$

$$\epsilon_n = \frac{\hbar^2}{8md^2} (n_1^2 + n_2^2 + n_3^2) = \frac{\hbar^2 k^2}{2m}$$

n = Quantum numbers

- Ground state E ; $n_1 = n_2 = n_3 = 1$ not zero!
- Degeneracy

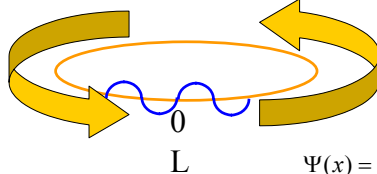
First excited state 112, 211, 121



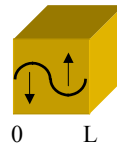
Consequence of Electrons as Waves on Free Electron Model



Traveling wave picture



Standing wave picture



$$\begin{aligned} \Psi(x) &= \Psi(x+L) \\ e^{ikx} &= e^{ik(x+L)} \\ e^{ikx} &= 1 \\ k &= \frac{2\pi n}{L} \end{aligned}$$

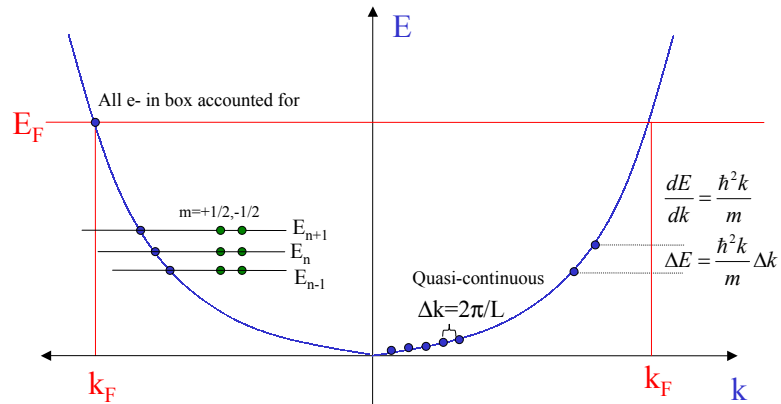
Just having a boundary condition means that k and E are quasi-continuous, i.e. for large L, they appear continuous but are discrete



Representation of E,k for 1-D Material

- states
- electrons

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



$$\text{Total number of electrons} = N = 2 * 2k_F * L / 2\pi$$

