Introduction of Nano Science and Tech

Quantum Effects in Nanostructures -Confinement and Coherence

Nick Fang

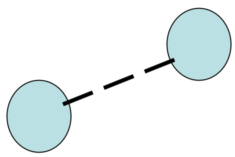
Course Website: **nanoHUB.org**
Compass.illinois.edu

Departure from continuum

- **Quantum Effects (Two Lectures)**
  - **Atomic bonding**
  - **Confinement**
  - **Coherence**
- **Basics of Kinetics and Statistical Thermodynamics (Two Lectures)**
  - **Microscopic Origin of Macroscopic Laws**
  - **Transport properties**

Quantum Effects

- How the energy are presented in discrete levels?



$$E_{translation} = \frac{\hbar^2 k^2}{2m}$$

$$E_{\text{Vibration}} = h\nu(n + \frac{1}{2}); \nu = \frac{1}{2\pi}\sqrt{\frac{K}{m}}$$

$$(n=0,1,2\cdots)$$

$$E_{\text{Rotation}} = hBl(l+1) \quad (l=0,1\cdots)$$

Solution of a Confined 1D system

- From the above boundary conditions, we obtain:

$$\sin(kD) = 0; \qquad k_n D = n\pi$$

(n=0, ±1, ± 2, …) the probability of the particles can only take standing wave forms!

Recall:

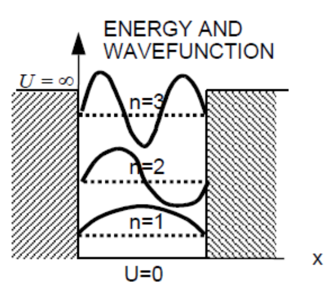
$$k = \frac{\sqrt{2mE}}{\hbar}$$

Finite Energy steps:

$$E_n = \frac{n^2 \hbar^2 \pi^2}{2mD^2}$$

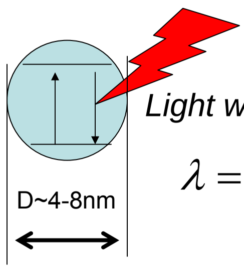
When D=1nm, m_e=9.1x10^{-31}kg

E_2-E_1=1.13eV!



Example: Quantum Dots

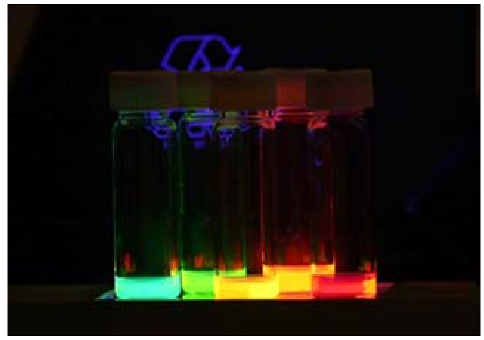
Quantum dots of the same material, but with different sizes, can emit light of different colors.



Light wavelength

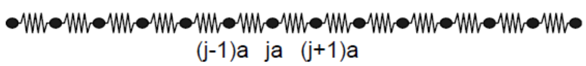
$$\lambda = \frac{hc}{\Delta E}$$

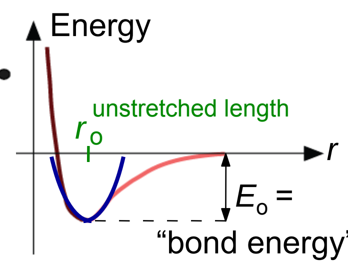
$$\frac{\partial \lambda}{\partial D} \propto \frac{16 m_e^* c}{h} D$$



http://en.wikipedia.org/wiki/Quantum_dots

Lattice Vibration, Phonon





$$m\frac{d^2u_j}{dt^2} = K(u_{j+1} - u_j) - K(u_j - u_{j-1}).$$

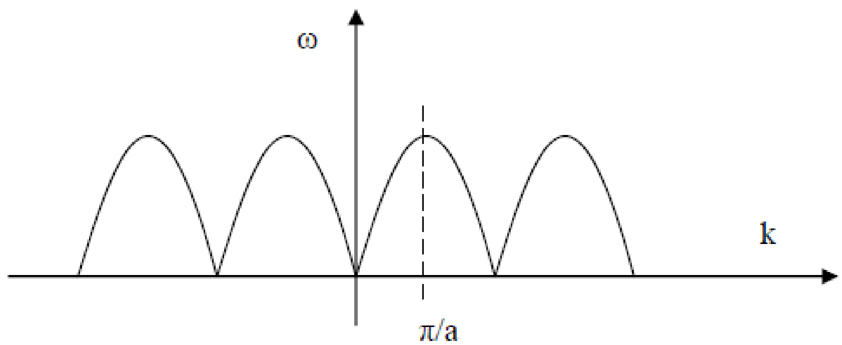
We attempt the following solution for the above equations of motion:

$$u_j = A\exp[-i(\omega t - kja)].$$

$$-m\omega^2 = K\left[e^{ika} + e^{-ika} - 2\right]$$

$$\omega = 2\sqrt{\frac{K}{m}}\left|\sin\frac{ka}{2}\right|.$$

Phonon Energy Diagram



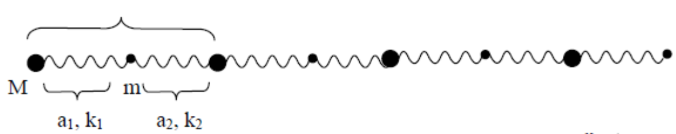
$$E_{vibration} = \hbar\omega(n + \tfrac{1}{2})$$

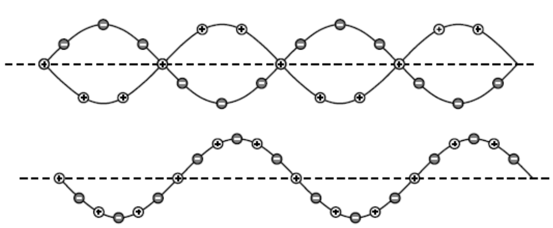
(n=0, ±1, ± 2, …)

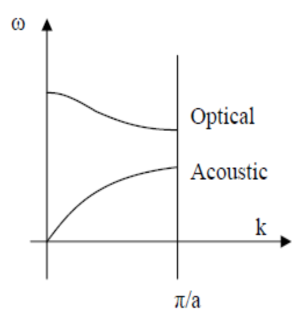
$$\omega = 2\sqrt{\frac{K}{m}}\left|\sin\frac{ka}{2}\right|.$$

ME 498 7

Polyatomic Lattice







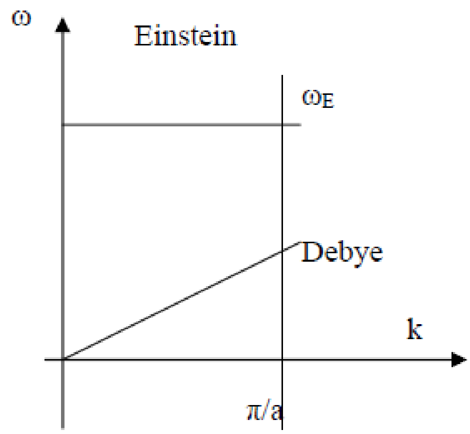
ME 498 8

Approximations

Einstein assumed a uniform vibration frequency for all atoms; the frequency is independent of momentum

Debye assumed the relationship between energy and momentum is completely **linear**

Both had some success explaining thermal capacity of solids



ME 498 9

Total Energy by Carriers

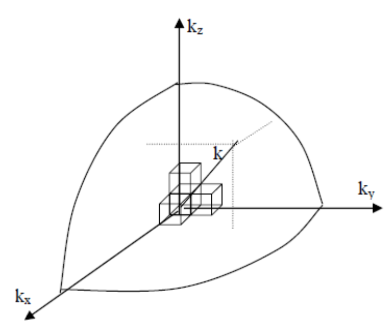
For example, what is the total internal energy carried by electrons?

We now know that the energy carried by each electron is

$$E_e = \frac{\hbar^2 k_e^{\,2}}{2m_e}$$

To find out the total energy carried, we can first assume the electrons move freely in all possible directions, or k_x, k_y, k_z can take arbitrary values.

$$k_{x,j} = \frac{j\pi}{L_x}$$



ME 498 10

Density of States (DOS)

For math convenience, we introduce a measure of the number of available quantum mechanical states per unit volume. This is typically measured at a specified energy E or momentum k.

E.G. the number of states within k and k+dk is

$$D(k)dk = \frac{4\pi k^2 dk}{V}$$

Convert this to the number of states within E and E+dE:

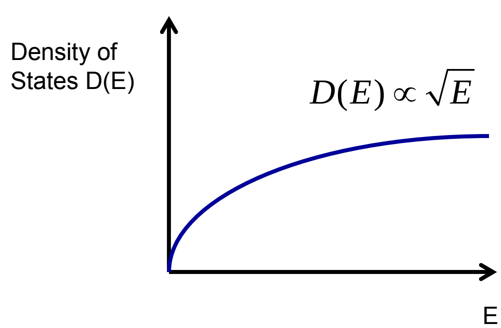
$$D(E)dE = \left(\frac{4\pi k^2}{V}\right)\left(\frac{dk}{dE}\right)dE$$

Since $k = \frac{\sqrt{2mE}}{\hbar}$ $\quad \frac{dk}{dE} = \frac{\sqrt{m/2E}}{\hbar}$

For bulk material we obtain:

$$D(E)dE = \frac{1}{V}\left(\frac{\sqrt{2m}}{\hbar}\right)^3\left(\sqrt{E}\right)dE$$

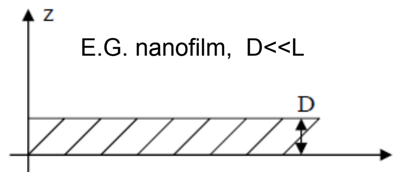
Electron Density of States (Bulk)

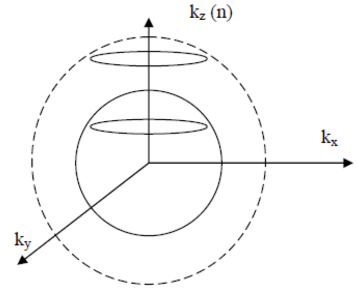


Importance:

Knowing the density of states allows us to find out the total internal energy, heat capacity, etc

Density of State in Nanostructures



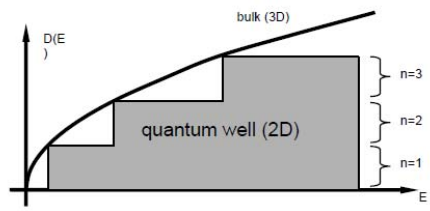


$$k_z = n\pi / D >> \pi / L$$

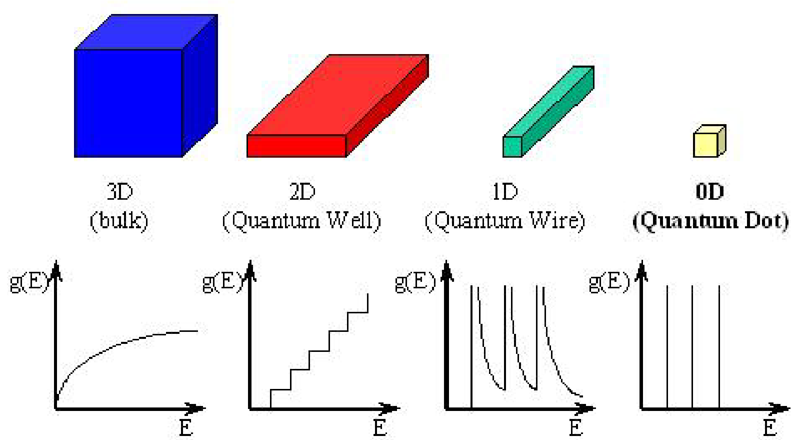
Therefore, k_x, k_y nearly continuous, but k_z discrete!

$$D(k_{xy}, n)dk = \frac{2\pi k dk}{V}$$

$$D(E, n)dE = C(n)dE$$

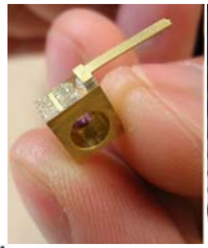


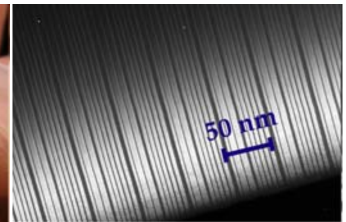
Density of States in Low Dimensions

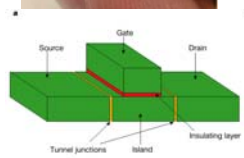


Application Examples

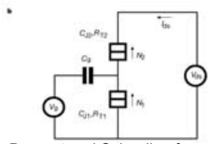
Quantum Cascade Laser (Bell Labs, 1994):







Single electron transistors

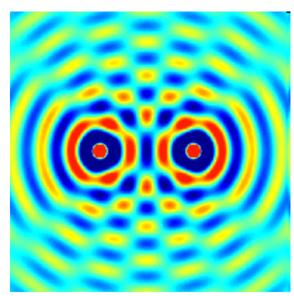


Devoret and Schoelkopf
Nature 406, 1039(2000)

Waves and Coherence

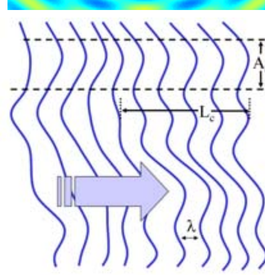
As the energy carriers are described by QM waves, energy flux is influenced by interference

i.e. $(A+B)^2 \neq A^2+B^2$



The capability of the carriers to interfere in a given system is defined as coherence:

$$\langle A(x_1,t_1) | B(x_2,t_2) \rangle$$

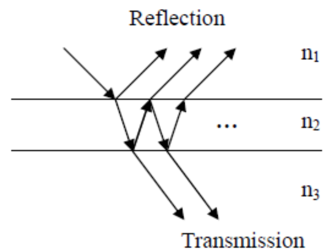


Size Effect

E.G. Reflection of light on a thin film

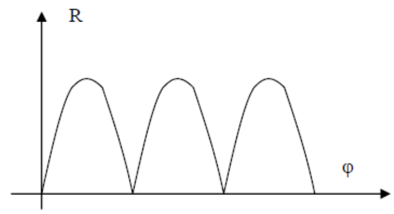
$$r = \frac{E_r}{E_i} = \frac{r_{12} + r_{23}\exp[2i\varphi_2]}{1 + r_{12}r_{23}\exp[2i\varphi_2]},$$

$$\varphi = k_z d$$



Note: R is maximized when

$$d = \pi / k_z(E)$$



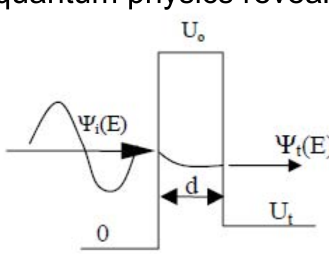
For 0.5eV electron, this is about 1.2nm

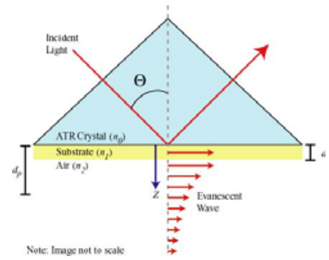
0.5eV photon, this is ~ 120nm

ME 498 17

Tunneling

Classical physics would predict that no particles with energy $E<U_0$ are transmitted;
quantum physics reveals that the probability of transmission





In optics, it is called evanescent waves:

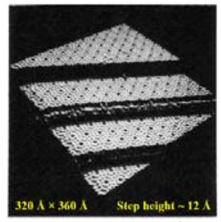
$$E_z(x,y,z) = E_0 \exp\left(ik_x x + ik_y y - \gamma z\right)$$

$$\gamma = \sqrt{k_x^2 + k_y^2 - \left(\frac{2\pi n_3}{\lambda}\right)^2}$$

ME 498 18

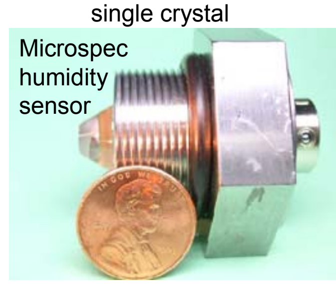
Applications of Tunneling

E.G. Scanning Tunneling Microscope (STM) invented by G. Binnig and H. Rohrer in 1982 (Nobel Prize in Physics, 1986)



Atomic image of silicon single crystal

E.G. Attenuated Total Internal Reflection (ATR) Sensor (commercial products such as GE BiaCORE provide ppm sensitivity)



http://www.sensorsportal.com/HTML/DIGEST/december_02/MicroSpec_Sensor.jpg

Additional Reading

- Tien, Majumdar, Gerner, "Microscale Energy Transport", Chapter 1, Taylor&Francis (pdf online)
- Introduction to Scanning Tunneling Microscopy on nanoHUB:

