Introduction of Nano Science and Tech

Basic Carrier Interactions in Nanostructures

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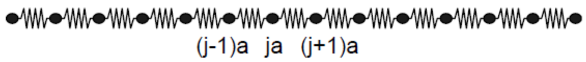
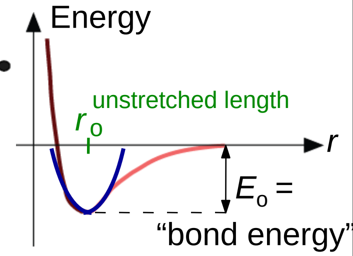
Course Website: **nanoHUB.org**
Compass.illinois.edu

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**

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:

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

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

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

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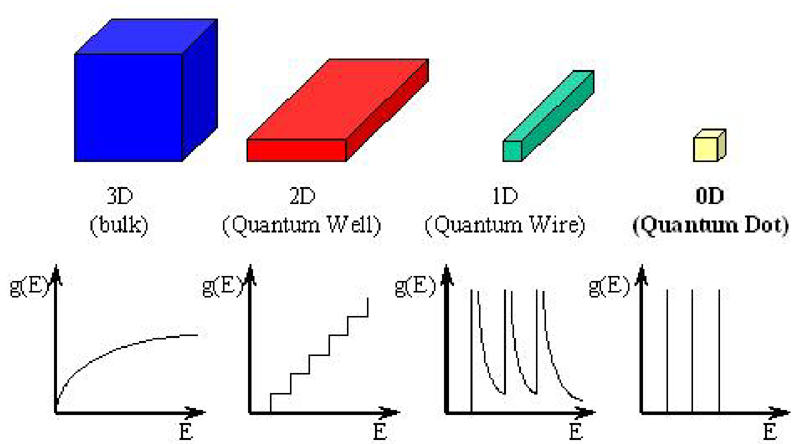
Density of States in Low Dimensions



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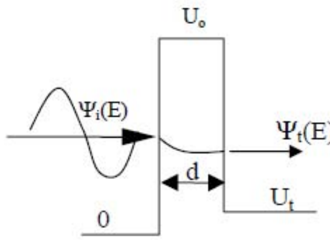
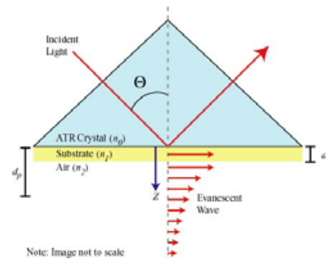
Tunneling

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:

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

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

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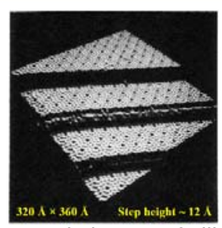
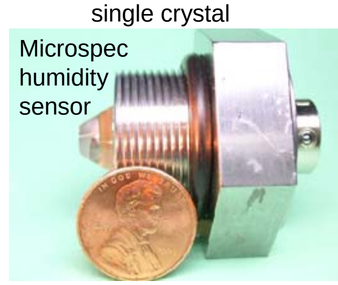
Applications of Tunneling

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

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Microscopic Transport Theory

To understand nanoscale transport and energy conversion, we need to know:

— **How much energy/momentum can a particle have?**

— **How many particles have the specified energy E?**

— **How fast do they move?**

— **How do they interact with each other?**

— How far can they travel?

Proportion of Particles at Given State

- Statistical thermodynamics gives the possibility p_i of finding a particle at given energy E_i:

$$p_i = \frac{e^{-E_i/k_B T}}{\sum_i e^{-E_i/k_B T}}$$

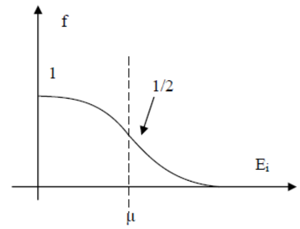
- E.G. for monatomic ideal gas, we only need to consider the kinetic energy

$$E = \frac{m}{2}\left(v_x^2 + v_y^2 + v_z^2\right) \qquad p(v) = \left(\frac{m}{2\pi\kappa_B T}\right)^{3/2} \exp\left[-\frac{m\left(v_x^2 + v_y^2 + v_z^2\right)}{2\kappa_B T}\right]$$

For Quantum Particles

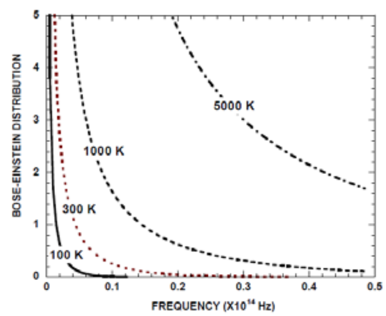
- Electrons: only two states possible (conduction, valence)

$$p(E_i) = \frac{\exp(-E_i / k_B T)}{1 + \exp(-E_i / k_B T)}$$



- Photons and Phonons: all possible states of energy $n\hbar\omega$

$$p(n) = \frac{\exp(-n\hbar\omega / k_B T)}{\sum \exp(-n\hbar\omega / k_B T)}$$



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How Fast do they move?

- Let's calculate the average kinetic energy

$$\langle E \rangle = \int_{-\infty}^{\infty} dv_x \int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} \frac{m}{2}\left(v_x^2 + v_y^2 + v_z^2\right) \; p(v_x, v_y, v_z) dv_z$$

- For monatomic gas

$$\langle E \rangle = \frac{3}{2} k_B T$$

At room temperature (300 K), this average energy is 39 meV, or 6.21×10^{-21} J.

For He gas, m=6.4x10^{-27} kg, v~1000 m/s

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How to compute average…

If you want to derive the formula $m < \frac{\vec{v}^2}{2} >= \frac{3}{2} k_B T$ **yourself…**

Use the following help:

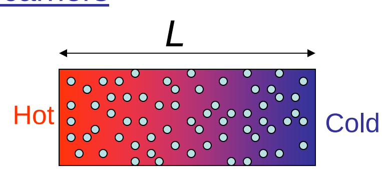
$$< \vec{v}_1^2 > = \int \vec{v}_1^2 \, P(\vec{v}_1, ..., \vec{v}_N) \, d\vec{v}_1 ... d\vec{v}_N$$

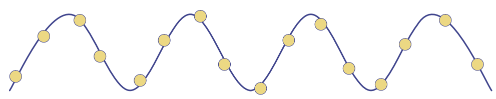
$$\vec{v}_1^2 = v_{1x}^2 + v_{1y}^2 + v_{1z}^2$$

$$d\vec{v}_1 = dv_{1x} \, dv_{1y} \, dv_{1z}$$

Interaction Between Carriers

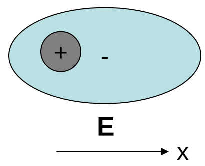
Materials	Dominant energy carriers
Gases:	Molecules
Metals:	Electrons
Insulators:	Phonons (crystal vibration)





- The collision of these particles can be of elastic or inelastic nature
- Energy and momentum transfer takes place

Photon Excitation in Materials



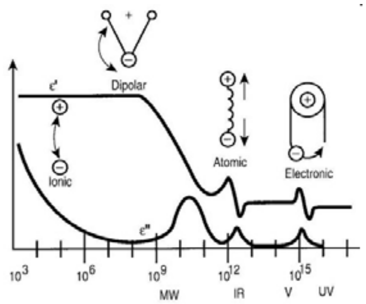
Lorenz Oscillator Model:

$$m\frac{\partial^2 x}{\partial t^2}+\gamma\frac{\partial x}{\partial t}+kx=eE_x$$

Molecular Polarizability $P_x = ex$ $\quad \varepsilon = 1 + n\frac{P}{\varepsilon_0 E}$

$$x=\frac{eE_x}{m(\omega_0^2-\omega^2+i\gamma\omega/m)}$$

$$\varepsilon = 1+\frac{ne^2}{\varepsilon_0 m}\left(\frac{1}{\omega_0^2-\omega^2+i\Gamma\omega}\right)$$



http://en.wikipedia.org/wiki/Permittivity #Complex_permittivity

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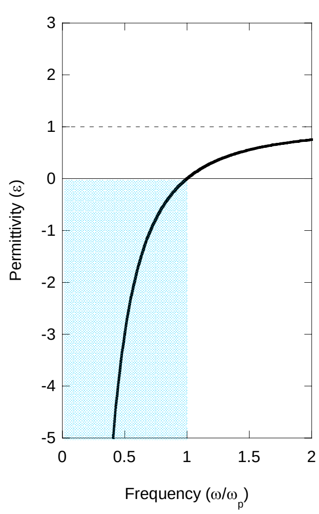
Photon-Electron Interactions



Drude Model: Free electron, restoring force =0

$$\varepsilon = 1-\frac{\omega_p^2}{\omega(\omega+i\gamma)}, \qquad \omega_p^2=\frac{n_e e^2}{\varepsilon_0 m_e}$$

When $\varepsilon<0$:

- Material is highly reflecting, no radiation allowed inside
- Magnetic field are expelled outside the material, field enhancement at the surface
- Surface mode (Surface Plasmon)

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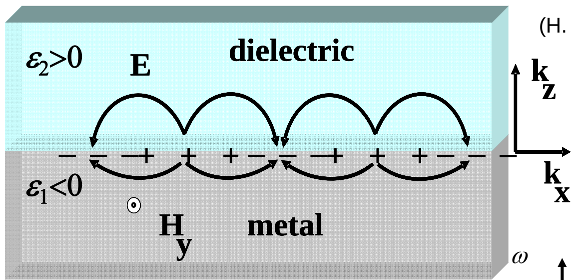
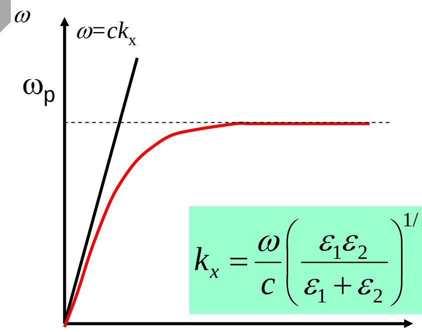
Surface Plasmons



(H. Raether, *Surface Plasmons*, Springer-Verlag, 1988)

- EM waves propagating along the interface between two media with their ε of opposite sign.
- Intensity maximum at interface; exponentially decays away from the interface.



$$k_x = \frac{\omega}{c}\left(\frac{\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}\right)^{1/2}$$

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Excitation of Surface Plasmons

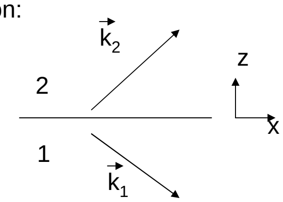
- consider a p-polarized wave propagates in x direction:

Z>0 $H_2 = (0,H_{y2},0)\exp(i(k_{x2}x+k_{z2}z-\omega t))$

$E_2 = (E_{x2},0,E_{z2})\exp(i(k_{x2}x+k_{z2}z-\omega t))$

Z<0 $H_1 = (0,H_{y1},0)\exp(i(k_{x1}x-k_{z1}z-\omega t))$

$E_2 = (E_{x1},0,E_{z1})\exp(i(k_{x1}x-k_{z1}z-\omega t))$



Boundary condition:

$E_{x1}=E_{x2}$, $H_{y1}=H_{y2}$, $\varepsilon_1 E_{z1}= \varepsilon_2 E_{z2}$

From above, we get:

$K_{x1}=k_{x2}=k_x$ $k_{z1}/\varepsilon_1= -k_{z2}/\varepsilon_2$

also, $k_{xi}^2 + k_{zi}^2 = \varepsilon_i(\frac{\omega}{c})^2$ ⟶

Dispersion relation:

$$k_x = \frac{\omega}{c}\left(\frac{\varepsilon_1\varepsilon_2}{\varepsilon_1+\varepsilon_2}\right)^{1/2}$$

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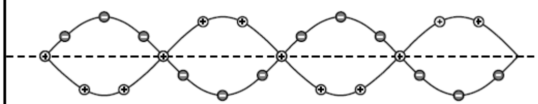
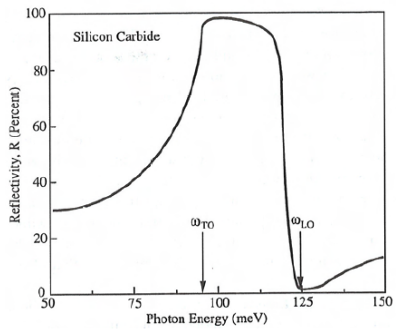
Photon-Phonon Interactions

- In polyatomic lattices, atoms of different mass can move in opposite directions: polarizable with light excitation

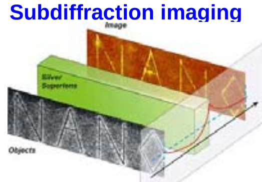


$$m_{eff} = \frac{m_1 m_2}{m_1 + m_2}$$



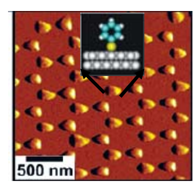
This excitation is often called phonon polaritons, and share many similar properties with plasmons, but appear at mid-IR wavelength (around 10 um)

Subdiffraction imaging



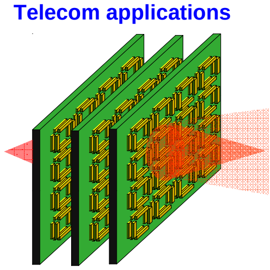
Fang *et al.*, Science, 2005

Sensing

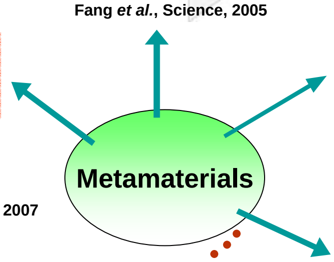


Van Duyne *et al.*, MRS bulletin, 2005

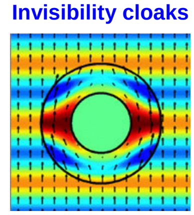
Telecom applications



Logeeswaran *et al.*, Appl. Phys. A, 2007



Invisibility cloaks



Chen *et al.*, PRL, 2007

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