Basic Carrier Interactions in Nanostructures

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Course Website: nanoHUB.org
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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

\[ E_0 = \| \text{"bond energy"} \]

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

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

\[ u_j = A \exp[-i(\omega t - k_j a)]. \]

\[ -m\omega^2 = K[e^{ika} - e^{-ika} - 2] \]

Density of States in Low Dimensions

- **3D (bulk)**
- **2D (Quantum Well)**
- **1D (Quantum Wire)**
- **0D (Quantum Dot)**

\[ g(E) \]
Tunneling

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

$$P(E) = \exp \left( -\frac{\gamma}{\lambda} \right)$$

In optics, it is called evanescent waves:

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

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

Applications of Tunneling

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

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

Microspec humidity sensor

http://www.sensorsportal.com/HTML/DIGEST/desember_02/MicroSpec_Sensor.jpg
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

$$ E = \frac{m}{2} \left( v_x^2 + v_y^2 + v_z^2 \right) $$

$$ P(v) = \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp \left[ -\frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T} \right] $$
For Quantum Particles

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

\[ p(E_i) = \frac{\exp(-E_i/k_BT)}{1 + \exp(-E_i/k_BT)} \]

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

\[ p(n) = \frac{\exp(-n\hbar\omega/k_BT)}{\sum \exp(-n\hbar\omega/k_BT)} \]

How Fast do they move?

- Let’s calculate the average kinetic energy

\[ \langle E \rangle = \int_{-\infty}^{\infty} d\nu_x \int_{-\infty}^{\infty} d\nu_y \int_{-\infty}^{\infty} m \left( \frac{\nu_x^2 + \nu_y^2 + \nu_z^2}{2} \right) p(\nu_x, \nu_y, \nu_z) d\nu_z \]

- For monatomic gas

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

At room temperature (300 K), this average energy is 39 meV, or 6.21x10^{-21} J.

For He gas, m=6.4x10^{-27} kg, \( v \sim 1000 \) m/s
If you want to derive the formula $m < \frac{v^2}{2} > = \frac{3}{2} k_B T$ 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

<table>
<thead>
<tr>
<th>Materials</th>
<th>Dominant energy carriers</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gases:</td>
<td>Molecules</td>
</tr>
<tr>
<td>Metals:</td>
<td>Electrons</td>
</tr>
<tr>
<td>Insulators:</td>
<td>Phonons (crystal vibration)</td>
</tr>
</tbody>
</table>

- 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

\[
P_x = ex \quad \varepsilon = 1 + n \frac{-Pe}{\varepsilon_0 E}
\]

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

\[
\varepsilon = 1 + \frac{n \epsilon_0^2}{\epsilon_0 m} \left( \frac{1}{\omega_0^2 - \omega^2 + i\Gamma \omega} \right)
\]

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**Photon-Electron Interactions**

**Drude Model:** Free electron, restoring force \(=0\)

\[
\varepsilon = 1 - \frac{\omega_p^2}{\omega \left( \omega + i\gamma \right)}
\]

\[
\omega_p^2 = \frac{n_e \epsilon_0 \epsilon_e}{\varepsilon_0 m_e e}
\]

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)
**Surface Plasmons**

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

\[ \omega = \frac{c k_x}{\varepsilon_1 + \varepsilon_2} \]

**Excitation of Surface Plasmons**

- Consider a p-polarized wave propagates in x direction:
  \[ Z>0 \quad H_z = (0, H_y, 0) \exp(i(k_x x + k_z z - \omega t)) \]
  \[ E_z = (E_{x1}, 0, E_{z1}) \exp(i(k_x x + k_z z - \omega t)) \]
  \[ Z<0 \quad H_z = (0, H_y, 0) \exp(i(k_x x - k_z z - \omega t)) \]
  \[ E_z = (E_{x1}, 0, E_{z1}) \exp(i(k_x x - k_z z - \omega t)) \]

Boundary condition:
- $E_{x1} = E_{x2}$, $H_{y1} = H_{y2}$, $\varepsilon_{z1} E_{z1} = \varepsilon_{z2} E_{z2}$

From above, we get:
- $k_x = k_{z1} = k_{z2}$
- $k_z = -i k_{z2} \varepsilon_{z1} / \varepsilon_{z2}$

also, $k_{z1}^2 + k_{z2}^2 = \varepsilon_{z1} \left( \frac{\omega}{c} \right)^2$

Dispersion relation:
\[ k_x = \frac{\omega}{c} \sqrt{\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2}} \]
Photon-Phonon Interactions

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

\[ m_{\text{eff}} = \frac{m_1 m_2}{m_1 + m_2} \]

This excitation is often called phonon polaritons, and share many similar properties with plasmons, but appear at mid-IR wavelength (around 10 \( \mu \text{m} \)).

Application: Metamaterials

- Subdiffraction imaging
  - Fang et al., Science, 2005
  - Van Duyne et al., MRS bulletin, 2005

- Sensing
  - Chen et al., PRL, 2007

- Invisibility cloaks

- Telecom applications

- Materials Today’s top 10 advances in material science over the past 50 years
- Discover top 100 science stories of the year 2006