Basics of Transport in Nanostructures

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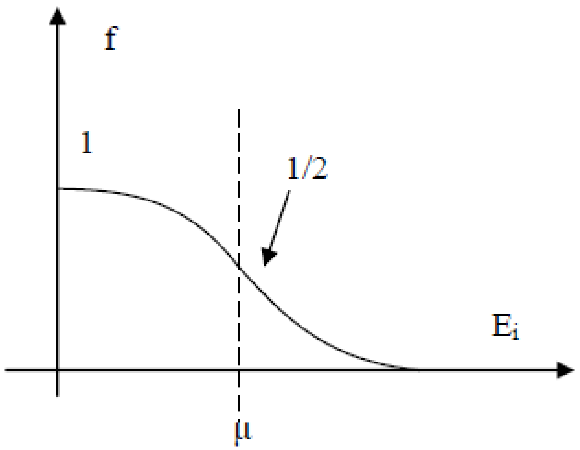
Course Website: **nanoHUB.org**
Compass.illinois.edu

For Quantum Particles

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

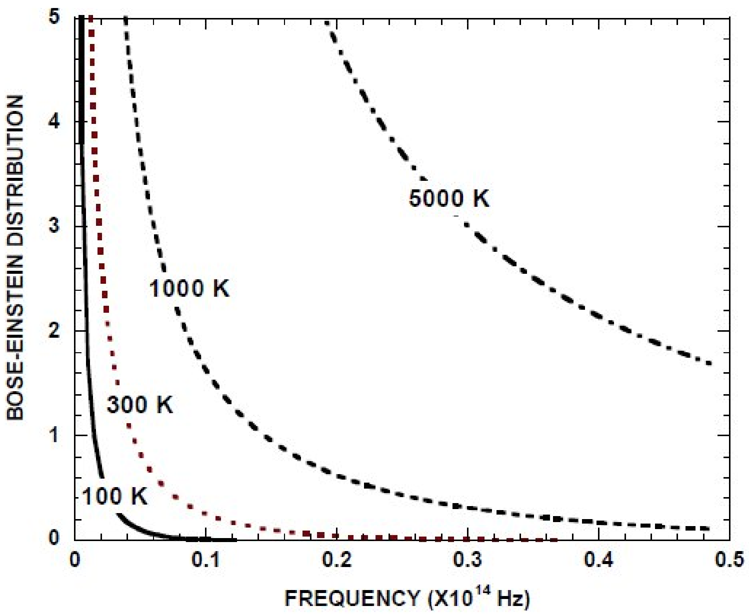
$$p(E_i) = \frac{\exp((E_F - E_i)/k_B T)}{1 + \exp((E_F - E_i)/k_B T)}$$



- Photons and Phonons: all possible states of energy

$$n\hbar\omega$$

$$p(\omega) = \frac{1}{\exp(\hbar\omega/k_B T) - 1}$$



How Fast do they move?

- Let's calculate the average kinetic energy

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

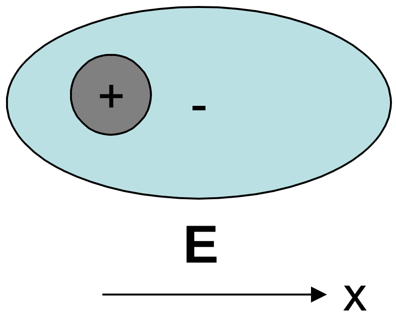
- For monatomic gas

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

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

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

Photon Excitation in Materials



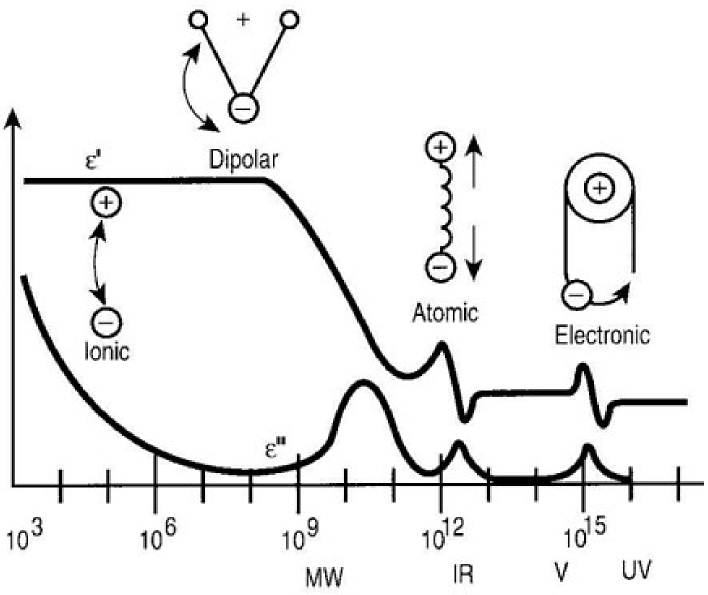
Lorenz Oscillator Model:

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

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

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

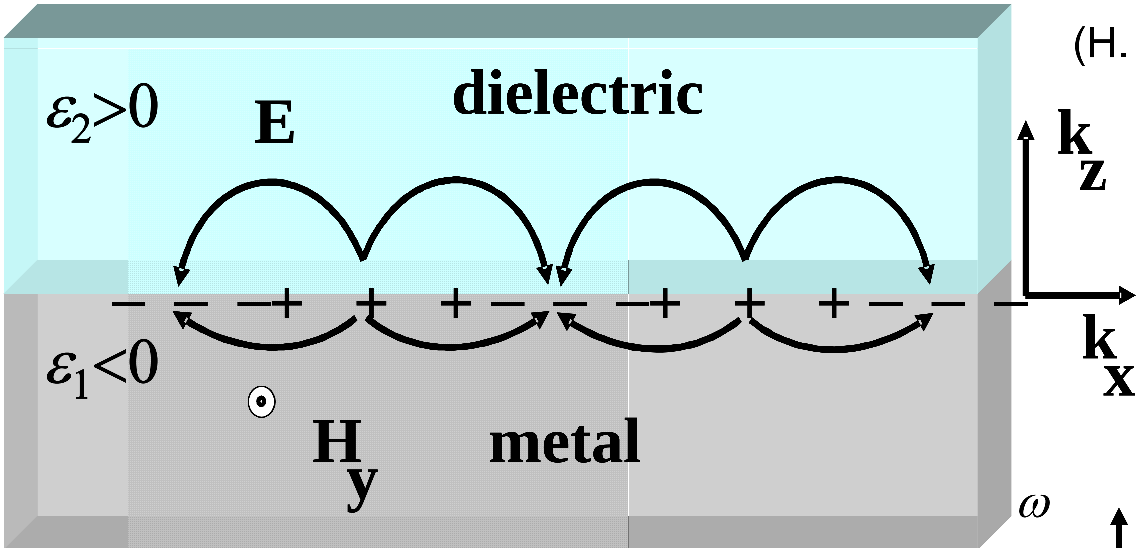
$$\varepsilon = 1+\frac{ne^2}{\varepsilon_0 m}\left(\frac{1}{\omega_0^2-\omega^2+i\Gamma\omega}\right)$$



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

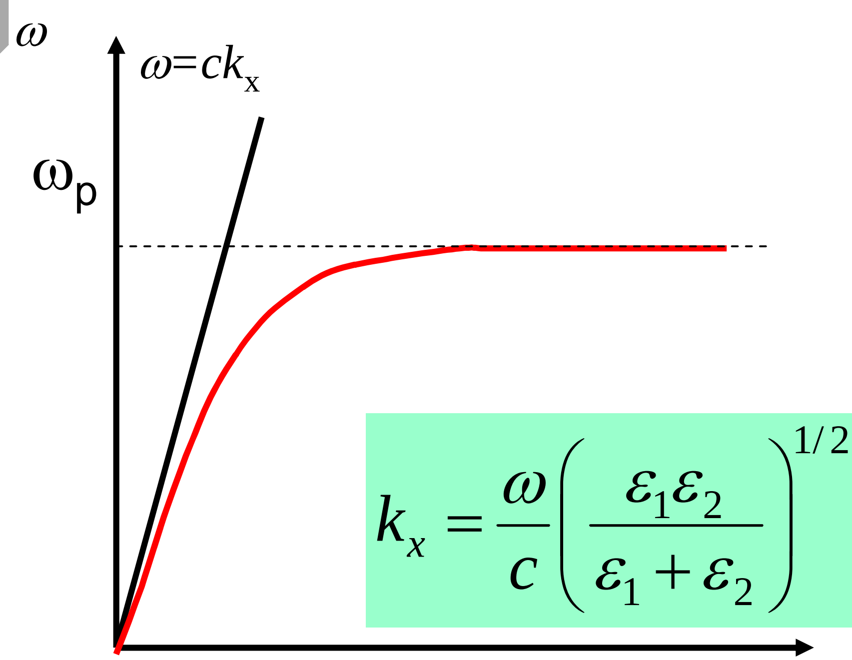
Surface Plasmons

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



- EM waves propagating along the interface between two media with their ε of opposite sign.

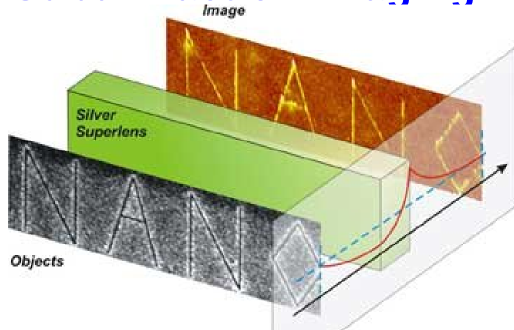
- Intensity maximum at interface; exponentially decays away from the interface.



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

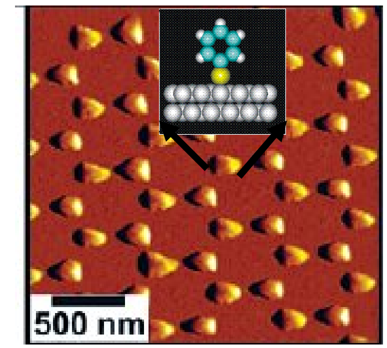
Application: Metamaterials

Subdiffraction imaging



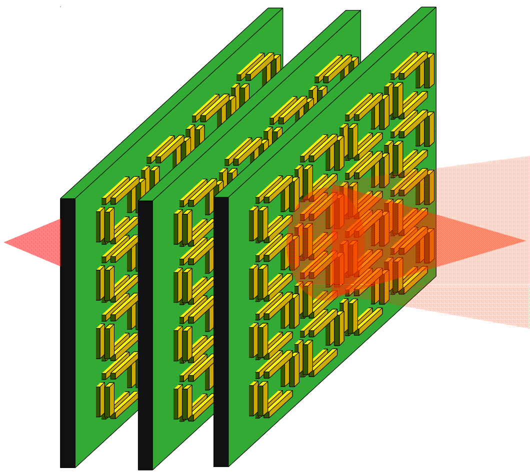
Fang *et al.*, Science, 2005

Sensing



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

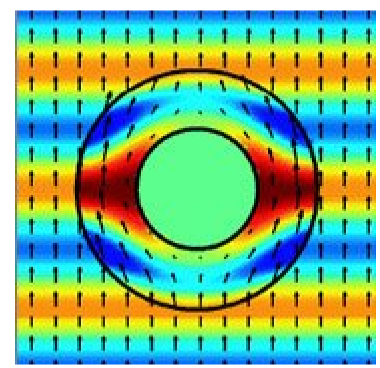
Telecom applications



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

Metamaterials

Invisibility cloaks



Chen *et al.*, PRL, 2007

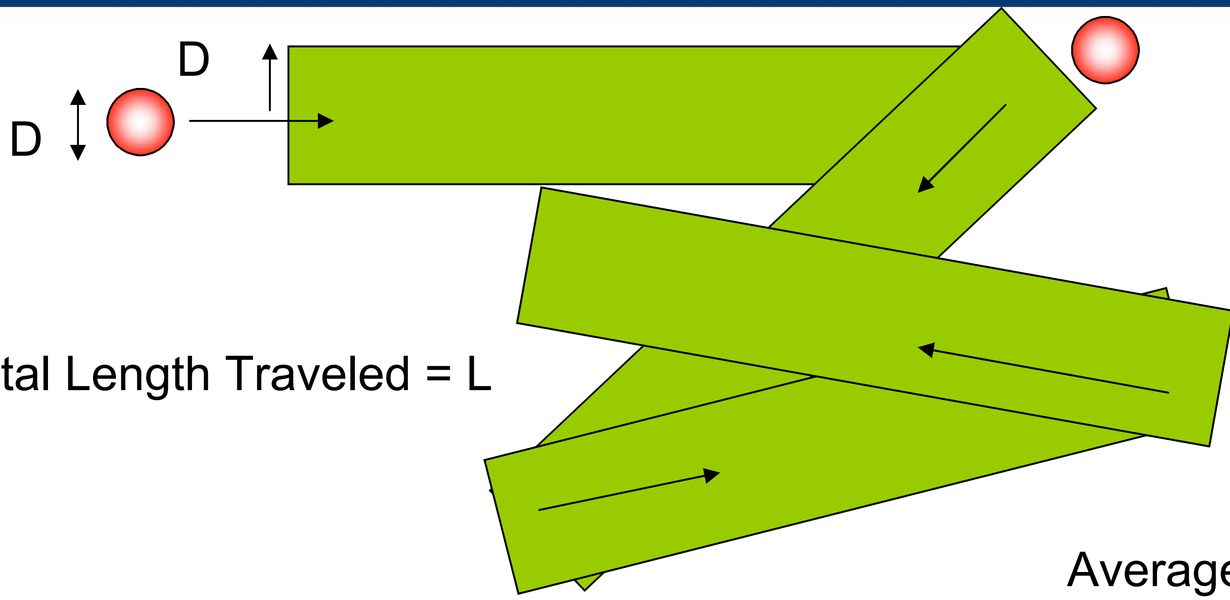
- ***Materials Today*'s top 10 advances in material science over the past 50 years**
- ***Discover* top 100 science stories of the year 2006**

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?**

How Far Can They Travel?



Total Length Traveled = L

Average Distance between Collisions, λ_{mc} = L/(#of collisions)

E.G. Ideal Gas:
Total Collision Volume Swept = $\pi D^2 L$

Number Density of Molecules = n

Total number of molecules encountered in swept collision volume ~ $n\pi D^2 L$

Mean Free Path

$$\lambda_{mc} = \frac{L}{n\pi D^2 L} = \frac{1}{n\sigma}$$

σ: collision cross-sectional area ~ **nm^2**

Mean Free Path for Gas Molecules

Number Density of Molecules from Ideal Gas Law: $\boldsymbol{n = P/k_B T}$

k_B: Boltzmann constant 1.38×10^{-23} J/K

Mean Free Path: $$\lambda_{mc} = \frac{1}{n\sigma} = \frac{k_B T}{P\sigma}$$

Typical Numbers:

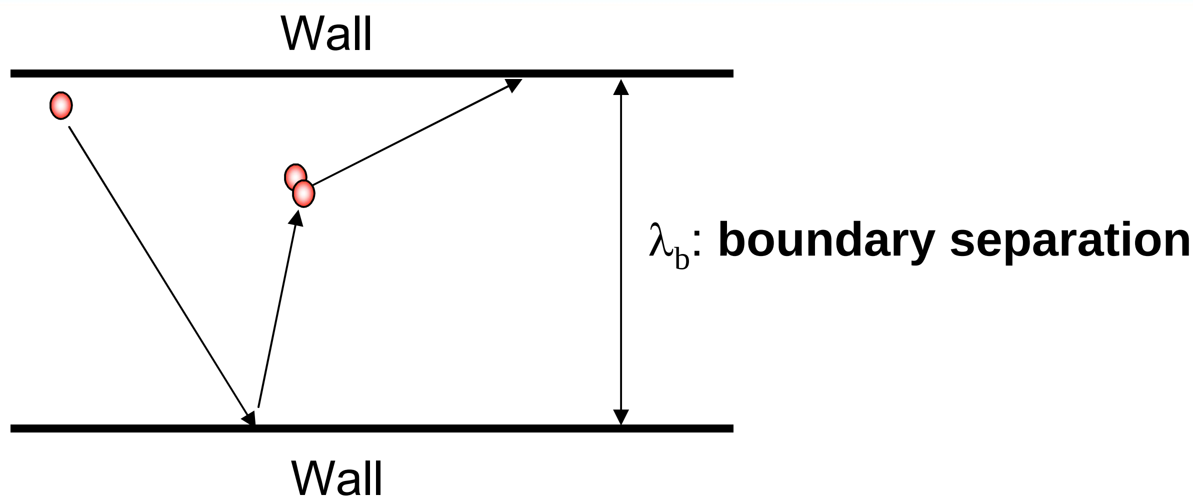
Diameter of Molecules, D ≈ 2 Å = 2 x10^{-10} m
Collision Cross-section: $\sigma \approx 1.3 \times 10^{-19}$ m^2

Mean Free Path at Atmospheric Pressure:

$$\lambda_{mc} \approx \frac{1.38 \times 10^{-23} \times 300}{10^5 \times 1.3 \times 10^{-19}} \approx 3 \times 10^{-7} \text{ m or } 0.3\mu\text{m}$$

At 1 Torr pressure, $\lambda_{mc} \approx 200$ μm; at 1 mTorr, $\lambda_{mc} \approx 20$ cm

Effect of Nanoscale confinement



Effective Mean Free Path:

$$\frac{1}{\lambda} = \frac{1}{\lambda_{mc}} + \frac{1}{\lambda_b}$$

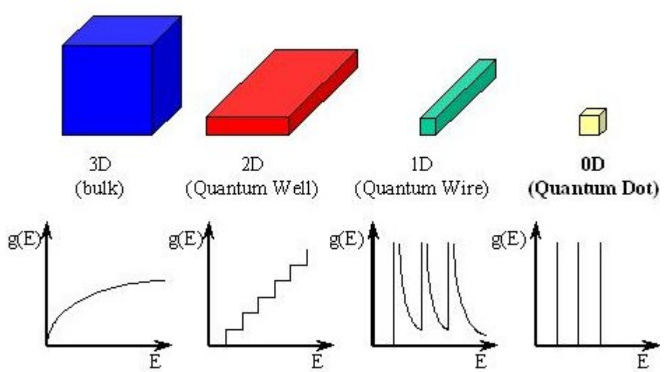
The smaller dimension governs collision time!

Internal Energy and Specific Heat

- Now we know the energy and momentum of particles/carriers in the material, we can start counting the properties
- E.G. Internal energy

Boltzmann Distribution — Density of States — Energy of Carrier at Given States

$$p_i = \frac{1}{Z} e^{-E_i/k_B T}$$



Translation

Vibration

Rotation

E.G. Internal Energy of Photons

Photon Energy at Given States

$$\hbar\omega = \hbar c k$$

In vacuum, 3D

Bose-Einstein Distribution

$$p(\hbar\omega) = \frac{1}{\exp(\hbar\omega / k_B T) - 1}$$

Density of States

$$D(\omega)d\omega = \frac{4\pi\omega^2}{Vc^3} d\omega$$

Total Internal Energy:

$$U = N\int_0^\infty \hbar\omega p(\omega) D(\omega) d\omega$$

Thermal Radiation (Planck's Law)

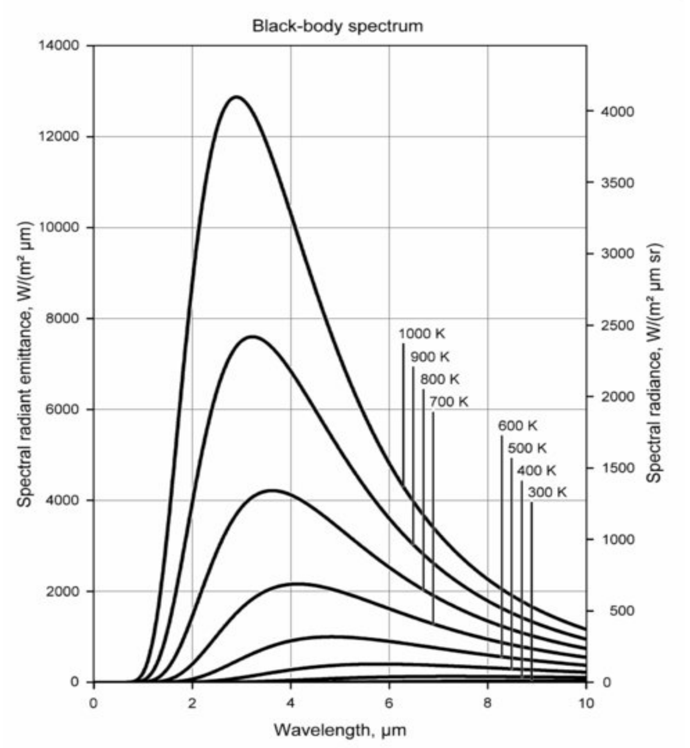
- Total Internal Energy of Vacuum Photons:

$$U = \frac{4\pi N}{Vc^3}\int_0^\infty \frac{\hbar\omega^3}{\exp(\hbar\omega/k_B T)-1}d\omega$$

Converting the distribution to wavelength, $\omega = \frac{2\pi c}{\lambda}$

$$P(\lambda) = -\frac{1}{\lambda^5}\frac{(2\pi\hbar c)^4}{\exp(2\pi\hbar c/\lambda k_B T)-1}d\lambda$$

describes the spectral radiance of electromagnetic radiation at temperature T.



http://upload.wikimedia.org/wikipedia/commons/8/85/BlackbodySpectrum_lin_150dpi_en.png

Thermal Radiation (Stefan-Boltzmann)

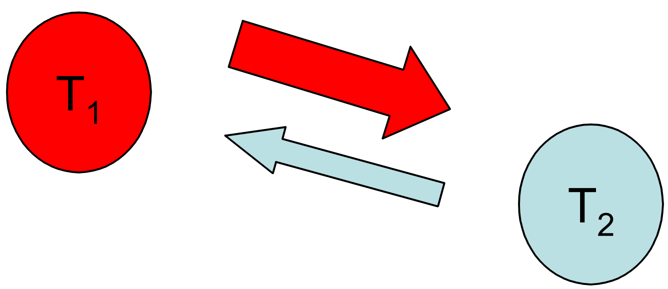
Define: $x = \mathrm{h}\omega / k_B T$

$$U(T) = \frac{4\pi N (k_B T)^4}{V(\mathrm{h}c)^3} \int_0^\infty \frac{x^3}{\exp(x) - 1} dx$$

The emissive power of Black body radiation:

$$E(T) = \sigma T^4$$

Stefan-Boltzmann's Law



$\sigma = 5.67 \times 10^{-8}\ \mathrm{W/m^2}\ K^4$.

$$q = \sigma \left(T_1^{\ 4} - T_2^{\ 4} \right)$$

Internal Energy of Phonons

- E.G. in a bulk solid

Phonon Energy at Given States

$$h\omega = h\sqrt{\frac{K}{m}}\sin(ka)$$

Boltzmann Distribution

$$p(\omega) = \frac{1}{\exp(h\omega/k_B T) - 1}$$

Density of States

$$D(\omega)d\omega \approx \frac{4\pi\omega^2}{V\left(a\omega_D\right)^{3/2}}d\omega$$

Debye Approximation

$$\omega < \omega_D = \sqrt{K/m}$$

Total Internal Energy:

$$U = 3N\int_0^{\omega_D} h\omega p(\omega)D(\omega)d\omega$$

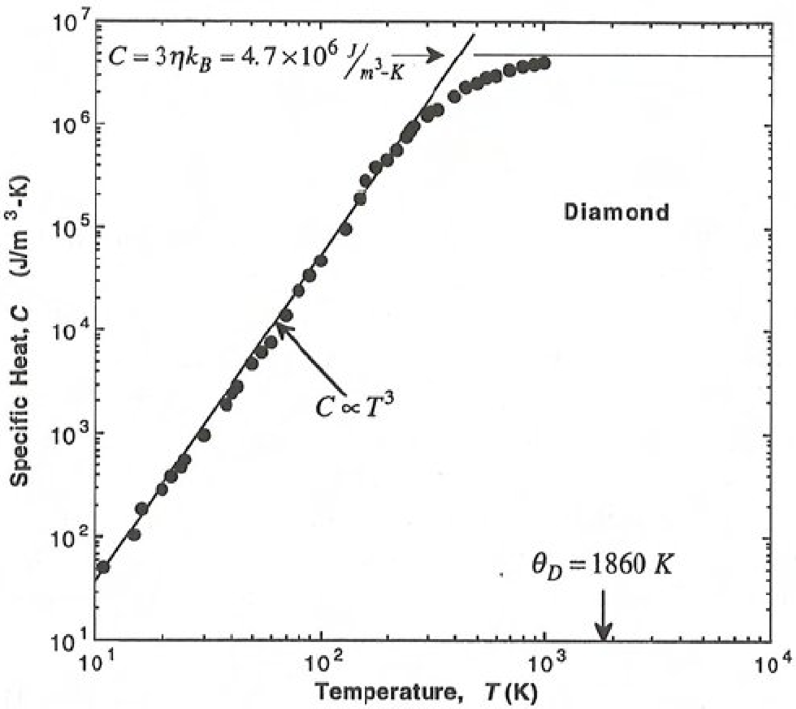
Specific Heat Capacity

- The specific heat capacity is defined by change of internal energy per unit temperature change:

$$C_V = \frac{\partial U}{\partial T}$$

$$U \propto T^4$$

$$\Rightarrow \quad C_V \propto T^3$$ At low temperature



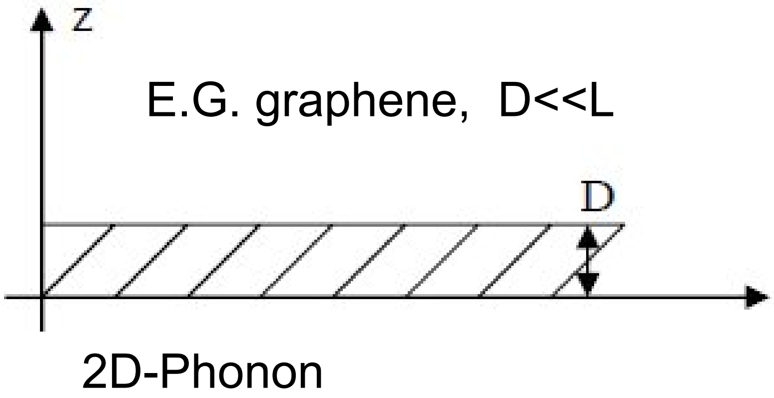
Specific heat of diamond

(Touloukian and Buyco, 1970).

Size Effect on Heat Capacity

Modified Density of States

$$D(\omega)d\omega \approx \frac{2\pi\omega(n)}{V\left(a\omega_D\right)}d\omega$$



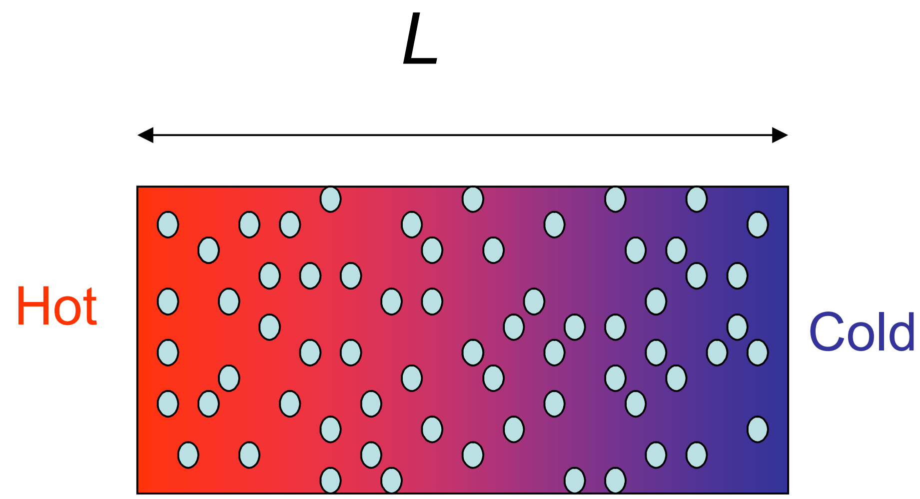
$$U \propto T^3 \qquad C_V = \frac{\partial U}{\partial T} \propto T^2 (film)$$

Nanoparticles:

$$U \propto T^{-1} \qquad C_V = \frac{\partial U}{\partial T} \propto T^{-2} \frac{\exp(T_E/T)}{(\exp(T_E/T)-1)^2}$$

Transport Properties

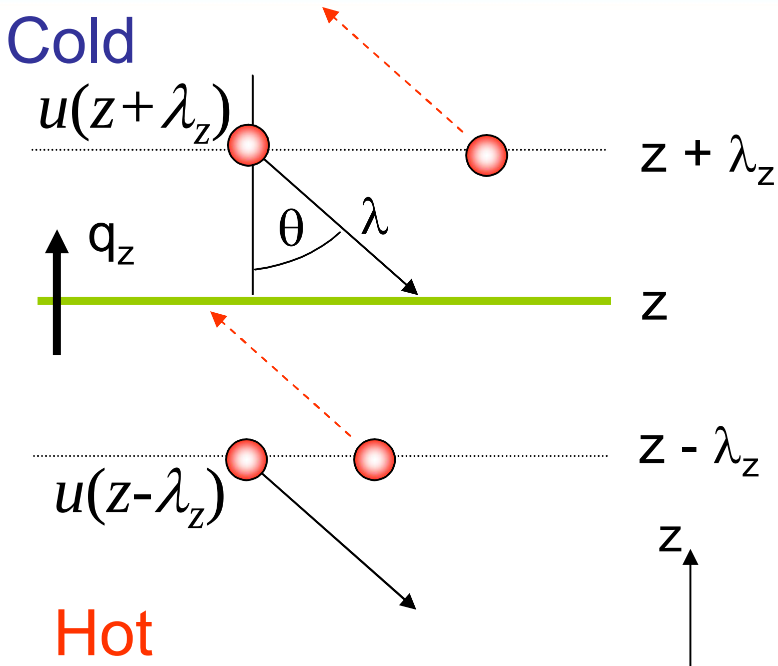
- E.G. Heat Conduction



In micro-nano scale thermal and fluid systems, often *L* < mean free path of collision of energy carriers & Fourier's law breaks down

→ Particle transport theories or molecular dynamics methods

Kinetic Theory of Energy Transport



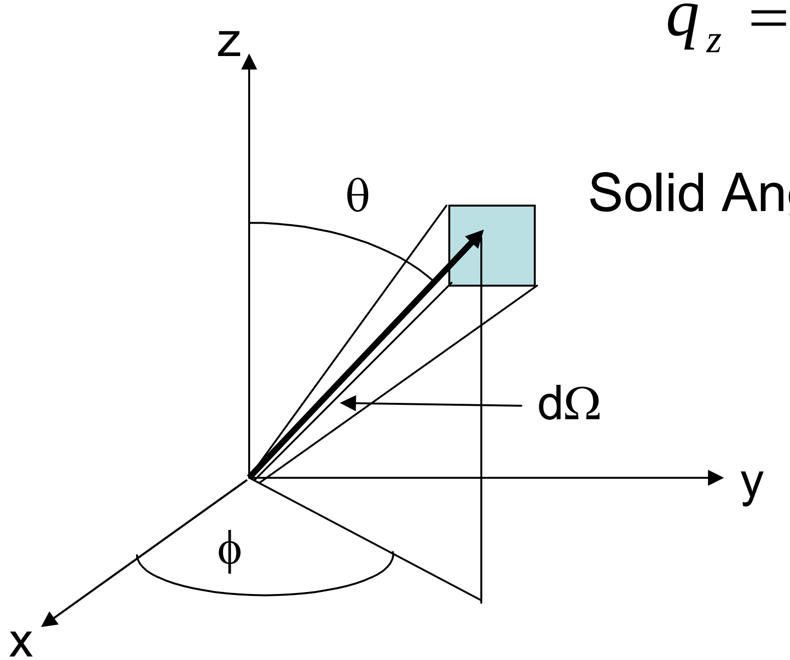
Net Energy Flux

$$q_z = \frac{1}{2} v_z \left[u(z - \lambda_z) - u(z + \lambda_z) \right]$$

through Taylor expansion of *u*

$$q_z = -v_z \lambda_z \frac{du}{dz}$$

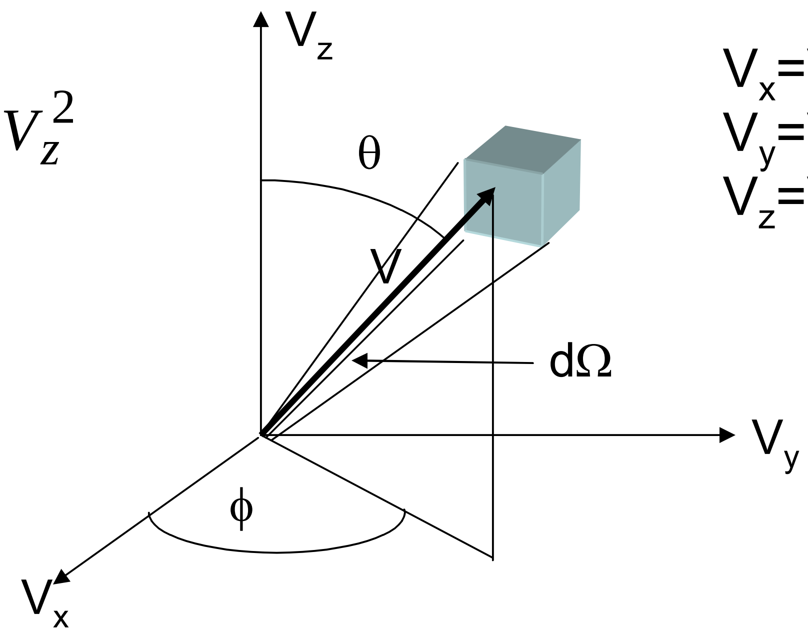
Solid Angle, $d\Omega = \sin\theta d\theta d\phi$



With a bit More Geometrics

Velocity:

$$V^2 = V_x^2 + V_y^2 + V_z^2$$



V_x=Vsinθcosϕ
V_y=Vsinθsinϕ
V_z=Vcosθ

$$q = -\left(\cos^2\theta\right) v \lambda \frac{du}{dz}$$

Averaging over all the solid angles

$$q_z = -v\lambda \frac{du}{dz}\left[\frac{\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi/2}\cos^2\theta\sin\theta\, d\theta\, d\varphi}{\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi/2}\sin\theta\, d\theta\, d\varphi}\right] = -v\lambda\frac{du}{dz}\left[\frac{\int_{\varphi=0}^{2\pi}\int_{\theta=0}^{\pi/2}\cos^2\theta\sin\theta\, d\theta\, d\varphi}{2\pi}\right] = -\frac{1}{3}v\lambda\frac{du}{dz}$$

Assuming **local thermodynamic equilibrium**: u = u(T)

$$q_z = -\frac{1}{3}v\lambda\frac{du}{dT}\frac{dT}{dz} = -\frac{1}{3}Cv\lambda\frac{dT}{dz}$$

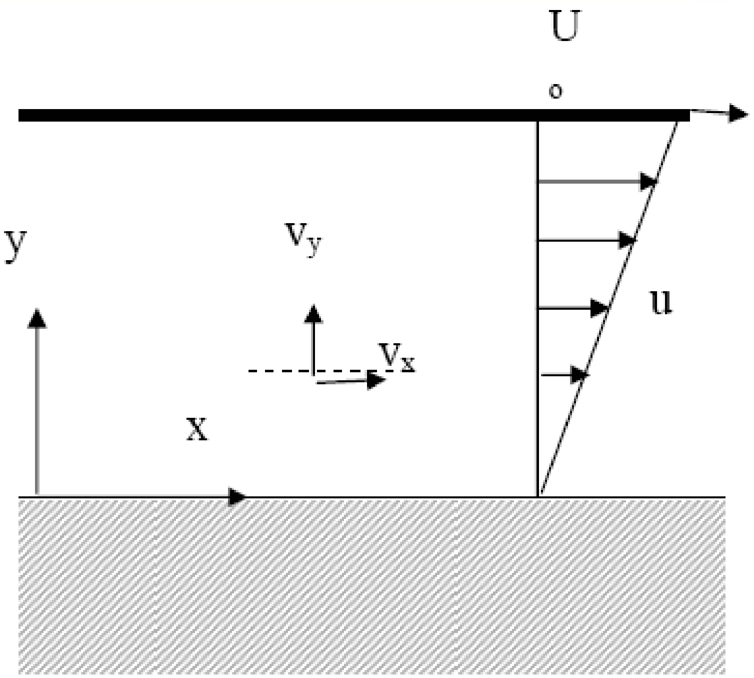
Thermal Conductivity

$$k = \frac{1}{3}Cv\lambda$$

Likewise…

- Newton's shear stress Law

$$\mu = l_{mc} \frac{n k_B T}{< v >}$$



$$P(v_x, v_y, v_z) = \left(\frac{m}{2\pi\kappa_B T} \right)^{3/2} e^{-m\left[(v_x - u)^2 + v_y^2 + v_z^2 \right] / 2\kappa_B T}$$

Additional Reading

- Tien, Majumdar, Gerner, “Microscale Energy Transport”, Chapter 1, Taylor&Francis (pdf online)

- ECE 598EP: Hot Chips: Atoms to Heat Sinks

http://poplab.ece.illinois.edu/teaching.html