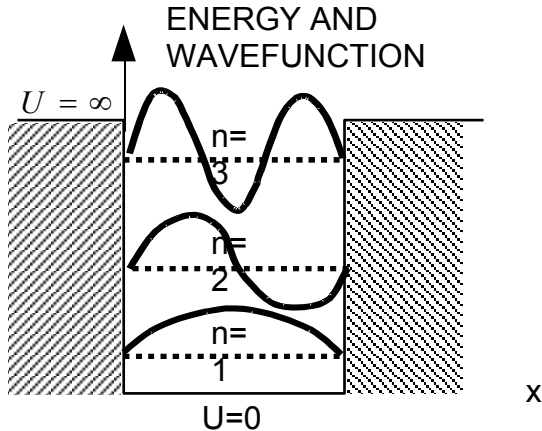


**2.57 Nano-to-Macro Transport Processes**  
**Fall 2004**  
**Lecture 9**

3.4 Density of states

(1) Electron in a quantum well



For electrons in a quantum well, the energy has discrete levels as

$$E = \frac{\hbar^2 n^2}{8m D^2} \quad (n=1,2,\dots)$$

For wavefunction  $\Psi_{n,s}$ , we have degeneracy  $g(n)=2$  due to the spin.

(2) Harmonic oscillator

The energy is

$$E_n = \hbar\nu(n + 1/2); \nu = \frac{1}{2\pi} \sqrt{\frac{K}{m}} \quad (n=0,1,2,\dots)$$

The wavefunction is  $\Psi_n$ , and the degeneracy is  $g(n)=1$ .

(3) Rigid rotation

The energy eigenvalues are

$$E_l = \frac{\hbar^2}{2I} \ell(\ell + 1) = \hbar B \ell(\ell + 1) \quad (\text{for } |m| \leq \ell, \ell = 0, 1, 2, \dots)$$

For wavefunction  $\Psi_{nlm}$ , the degeneracy is  $g(l)=2l+1$ .

(4) Hydrogen atom

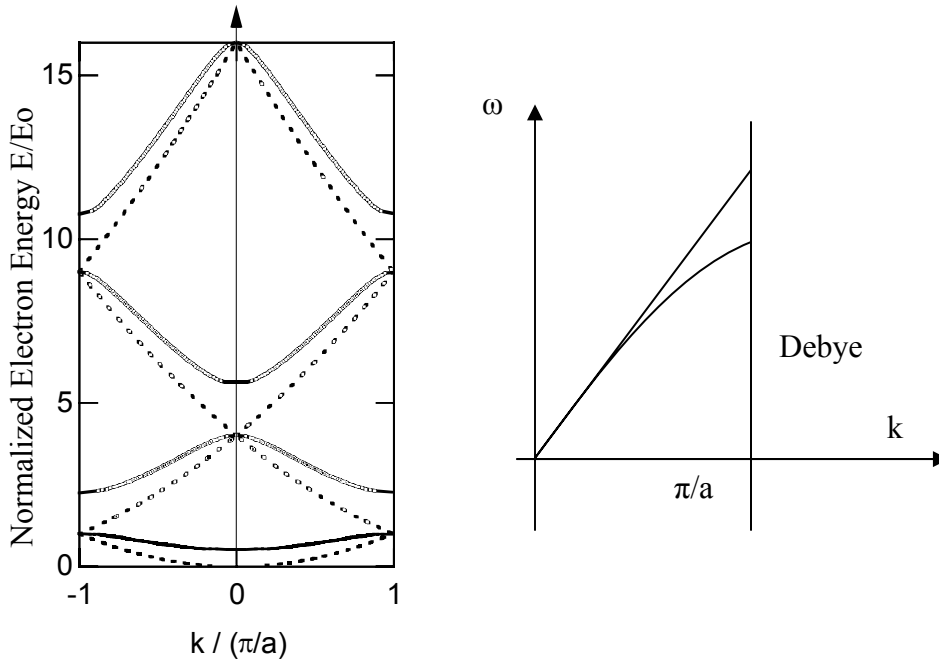
$$E_n^{el} = -\frac{Mc_1^2}{2\hbar^2 n^2} = -\frac{13.6 \text{ eV}}{n^2} \quad (n \geq 1, n \geq \ell + 1 \text{ and } |m| \leq \ell, \ell = 0, 1, 2, \dots)$$

The wavefunction  $\Psi_{nlms}$  corresponds to degeneracy  $g(n)=2n^2$ .

Now let us consider electrons in a solid. The parabolic approximation at the band edge gives

$$E - E_c = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m^*},$$

where  $k_x, k_y, k_z = \pm \frac{2\pi na}{L}$ . In different directions, n values can be different. For wavefunction  $\Psi(k_x, k_y, k_z)$ , we have three quantum numbers.



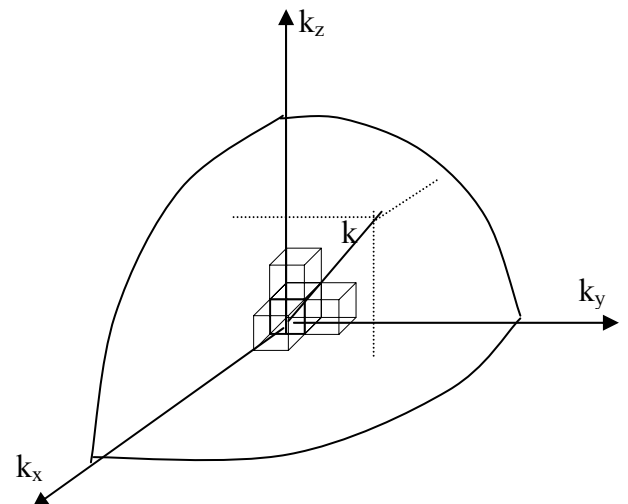
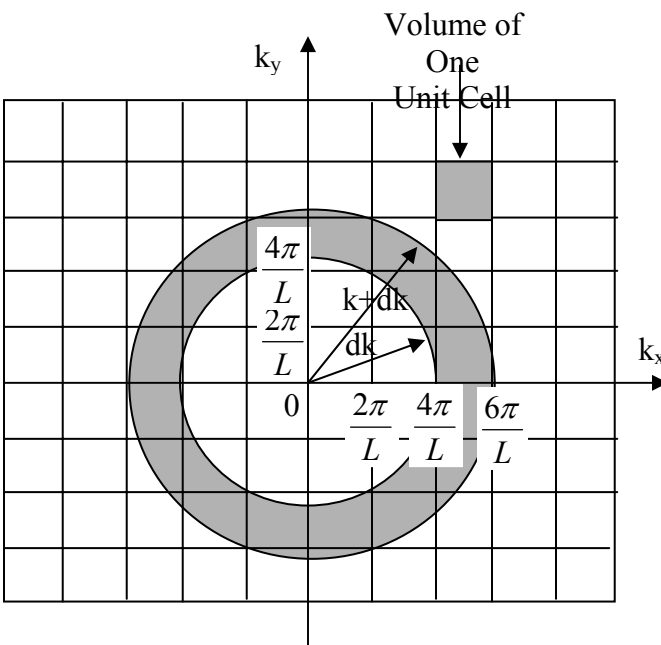
In the Debye approximation, we have energy dispersion as

$$\omega = vk = v\sqrt{k_x^2 + k_y^2 + k_z^2}; E_n = hv(n + \frac{1}{2}),$$

where  $v$  is sound velocity.

Density of (quantum mechanical) states (DOS):

(a) Electron



In above figure, we can find the volume of one state is  $V_1 = (2\pi/L)^3$ . In the above sphere, the number of states within  $k$  and  $k+dk$  is

$$\Delta N = \frac{4\pi k^2 \Delta k}{V_1} = \frac{V k^2 \Delta k}{2\pi^2},$$

in which  $V=L^3$  is the crystal volume.

The density of states is defined as the number of quantum states per unit interval of energy and per unit volume

$$D(E) = \frac{1}{V} \frac{\Delta N}{\Delta E} = \frac{k^2}{2\pi^2} \frac{\Delta k}{\Delta E} = \frac{k^2}{2\pi^2} \frac{dk}{dE}.$$

At the band edges, the electrons have energy

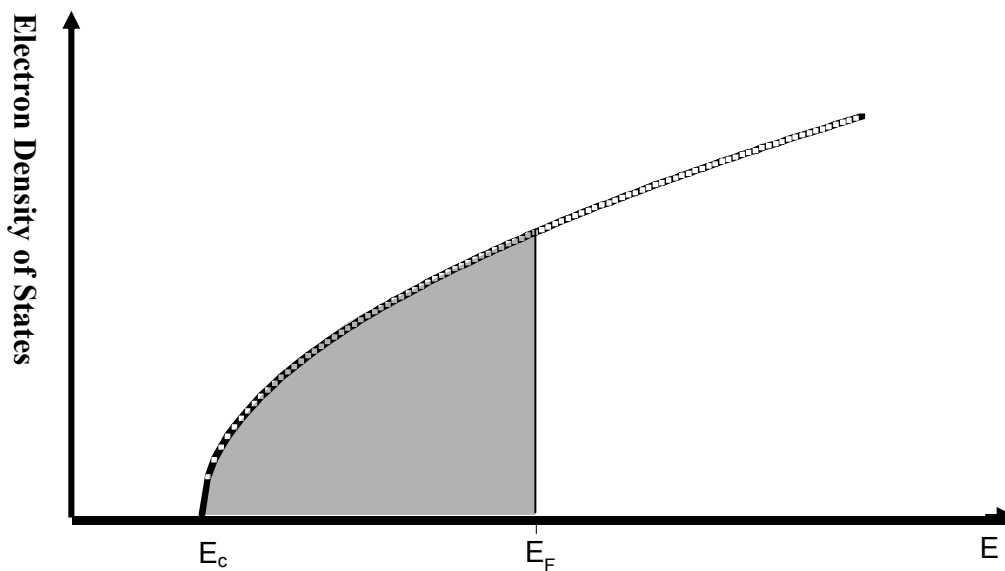
$$E = E_c + \frac{\hbar^2 k^2}{2m^*} = E_c + \frac{\hbar^2 (k_x^2 + k_y^2 + k_z^2)}{2m^*},$$

thus

$$k = \sqrt{\frac{2m^*}{\hbar^2} (E - E_c)}.$$

Considering spin, the density of states is

$$D(E) = 2 \frac{k^2}{2\pi^2} \frac{dk}{dE} = \frac{1}{2\pi^2} \left(\frac{2m^*}{\hbar^2}\right)^{3/2} (E - E_c)^{1/2}.$$



(b) Phonon

According to the Debye model that assumes three modes (two transverse, one longitudinal) are identical, we have

$$D(\omega) = 3 \frac{\Delta N}{V \Delta \omega} = \frac{3}{2\pi^2} k^2 \frac{dk}{d\omega} = \frac{3\omega^2}{2\pi^2 v^3}; \omega = vk.$$

(c) Photon

For electromagnetic waves, we only have two transverse modes. The density of states is

$$D(\omega) = \frac{\omega^2}{\pi^2 c^3}.$$

We may also want to use  $D(\lambda)$  in radiation problems.

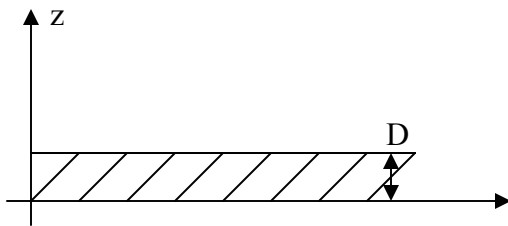
The density of states is a purely mathematical convenience but is central to correct counting of the number of electrons and the energy (or charge and momentum) that they carry. As a simple example of how the density of states is needed, let's evaluate the energy of the topmost level at  $T=0$ , i.e., the Fermi level,  $E_f$ . At zero Kelvin, the filling of the electron quantum states starts from the lowest energy level and moves up from one energy level to the next until all electrons are placed into distinct quantum states. The number of electrons per unit volume at  $T=0$  is

$$n = \int_{E_c}^{E_f} D(E) dE = \frac{1}{3\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} (E_f - E_c)^{3/2},$$

in which the electron density  $n=N/V$ .

For nonzero temperatures,  $E_f$  is replaced by the chemical potential.

Nanostructures:



For a thin film with thickness  $d$ , we have the energy as

$$E(k_x, k_y, n) = \frac{\hbar^2 k_{xy}^2}{2m^*} + n^2 \frac{\hbar^2 \pi^2}{2m^* d^2} \quad (n=1,2,\dots)$$

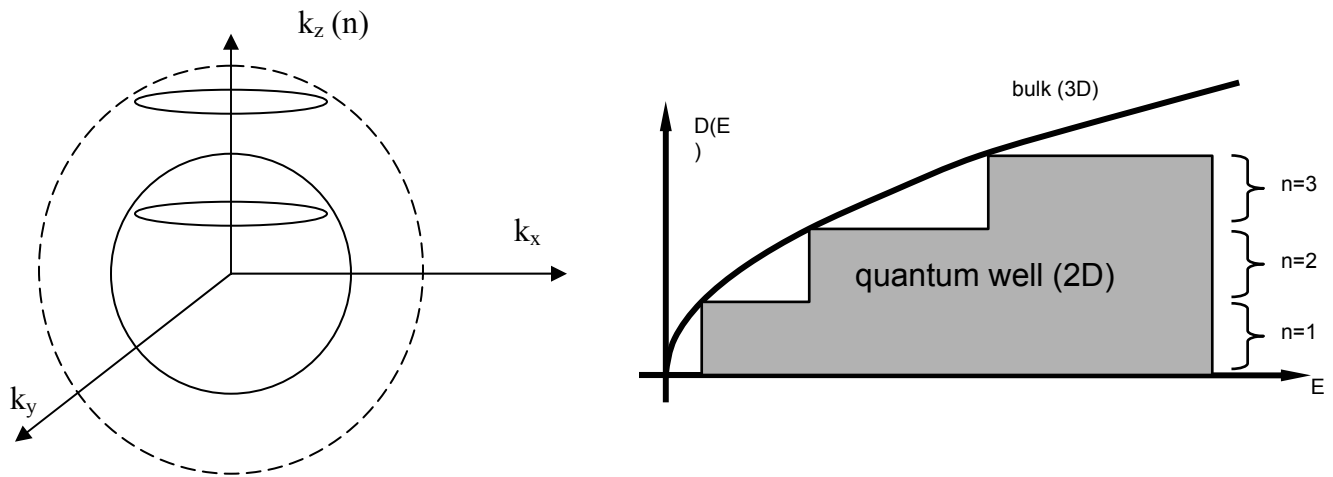
And we define  $E_n = n^2 \hbar^2 \pi^2 / (2m^* d^2)$  for convenience. In the  $k$  space,  $k_x, k_y = \pm \frac{2\pi ja}{L}$ ,

while the  $z$  direction is quantized by number  $n$ . For a given energy  $E$ , we have solutions for  $k_x, k_y$  when  $E_n < E$ . A constant energy surface is drawn in the following figure. Here we can nondimensionalize the coordinates to maintain the surface as a sphere. The solutions lie on the sketched circle determined by  $E - E_n$ , i.e.

$$|k_{xy}| = \sqrt{E(k_x, k_y, n) - E_n} \frac{\sqrt{2m^*}}{\hbar}.$$

If  $E_n > E$ , no solutions are available on this sphere. A large sphere corresponding to a higher  $E$  is required to find solutions for  $k_x, k_y$ .

The calculated density of states is presented in the following figure, which is staircase for one-dimensional constraint. For two-dimensional constraint (quantum wire in HW,  $n, l$  as the quantum numbers), we have  $D(E) \propto (E - E_{nl})^{-1/2}$ . If all three dimensions are under constraint (quantum dot,  $n, l, k$  as the quantum numbers), the density of states is just like jumps at different  $E_{nlk}$ .



#### Chapter 4 Statistical thermal & energy storage

In Lecture 2, we have mentioned that matter tends to occupy the lowest energy levels. For an energy level  $E_i$ , we have given the Boltzmann factor for its occupying probability as

$$P(E_i) = A \exp(-E_i / k_B T),$$

in which the constant  $A$  can be determined by normalization over all quantum states

$$\sum_{All\ QS} P(E_i) = 1.$$

For monatomic atom, we have

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

Normalization gives

$$A \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left[-\frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T}\right] dv_x dv_y dv_z = 1$$

$$A = \left(\frac{m}{2\pi k_B T}\right)^{3/2}.$$

The average number of particles is

$$f = \langle n \rangle = n \left( \frac{m}{2\pi k_B T} \right)^{3/2} \exp \left[ -\frac{m(v_x^2 + v_y^2 + v_z^2)}{2k_B T} \right]$$

where  $n$  is the particle number density. The Boltzmann factor can only be applied to closed systems, while for an open system exchanging energy with the outside, the probability becomes

$$P(E_i, N_i) = A \exp[-(E_i - \mu N_i) / k_B T],$$

where  $N_i$  is the particle number, chemical potential  $\mu$  is the criteria for the equilibrium state of mass exchanging process with the outside, just as pressure for mechanical equilibrium and temperature for thermal equilibrium.

Now consider electrons at energy  $E_i$ . Ignoring the spin, we have two possibilities:

Electron number	$N_i$	Energy $E_i$
0	0	0
1	1	$E_i$

Normalization gives

$$P(0, 0) + P(E_i, 1) = 1$$

or

$$A + A \exp[-(E_i - \mu) / k_B T] = 1.$$

Therefore

$$A = \frac{1}{1 + e^{-(E_i - \mu) / k_B T}}.$$

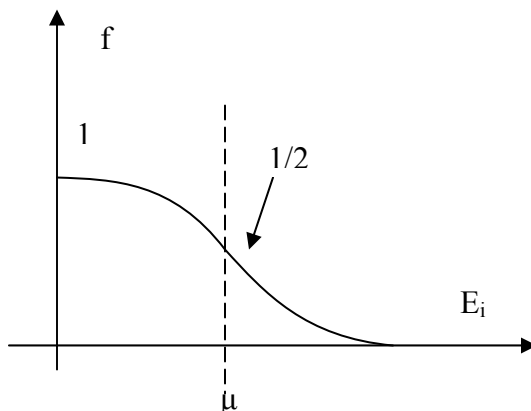
The average number of occupancy of this quantum state is thus

$$f = \langle n \rangle = 0 \times P(0, 0) + 1 \times P(E_i, 1)$$

$$= \frac{1}{1 + e^{-(E_i - \mu) / k_B T}} e^{-(E_i - \mu) / k_B T}$$

$$= \frac{1}{1 + e^{(E_i - \mu) / k_B T}}.$$

This is called the Fermi-Dirac distribution.



For phonons, the energy is expressed as

$$E_n = h\nu(n + \frac{1}{2}) \quad (n=0,1,2\dots)$$

Thus

$$\sum_{n=0}^{\infty} A \exp[-\frac{h\nu(n + 1/2)}{k_B T}] = 1$$

$$\exp(-\frac{h\nu}{2k_B T}) \sum_{n=0}^{\infty} A \exp(-\frac{h\nu n}{k_B T}) = 1$$

$$\exp(-\frac{h\nu}{2k_B T}) A \frac{1}{1 - \exp(-\frac{h\nu}{k_B T})} = 1.$$

$$A = \exp(\frac{h\nu}{2k_B T}) (1 - \exp(-\frac{h\nu}{k_B T})).$$

And

$$P(E) = \exp(-\frac{nh\nu}{k_B T}) [1 - \exp(-\frac{h\nu}{k_B T})].$$

Then the average number of the phonons, or the occupancy of the quantum state is

$$\begin{aligned} \langle n \rangle &= \sum_{n=0}^{\infty} n P(E_n), \\ &= [1 - \exp(-\frac{h\nu}{k_B T})] \sum_{n=0}^{\infty} n \exp(-nh\nu / k_B T) \\ &= [1 - \exp(-\frac{h\nu}{k_B T})] \left[ -\frac{d}{dx} \sum_{n=0}^{\infty} \exp(-nx) \right] \quad (x=h\nu/k_B T) \\ &= \frac{1}{e^{h\nu/k_B T} - 1} \end{aligned}$$

which is the Bose-Einstein distribution.

Note: The differentiation is a mathematical trick that leads to the same results as the original summation.