

# Discussion #5 Something related to HW #2

## Definition of density of states (DOS)

$$n = \frac{2}{V} \sum_{k_x} \sum_{k_y} \sum_{k_z} f_n(E) \equiv \int_0^{\infty} \rho_e(E) f_n(E) dE$$

$n$ : electrons per unit volume

$V$ : volume of interest

$2$ : accounts for spin degeneracy

$\sum_{k_x} \sum_{k_y} \sum_{k_z}$ : Summing over all possible states.  $k_x, k_y$  and  $k_z$  are wave numbers.  
(together they specify wave vectors)

$f_n(E)$  Fermi-Dirac distribution

$\rho_e(E)$ : DOS

★ Therefore, by re-writing  $\frac{2}{V} \sum_{k_x} \sum_{k_y} \sum_{k_z} f_n(E)$  in terms of energy  $E$ , we can find out the density of states  $\rho_e(E)$

★ Two different types of B.C.'s for electrons in a 3D box of dimensions  $L_x, L_y, L_z$

(a) 1st type of B.C.: Wavefunctions vanish at the surfaces of box.

$$\left. \begin{aligned} \therefore \phi(x=0) = \phi(x=L_x) = 0 \\ \phi(y=0) = \phi(y=L_y) = 0 \\ \phi(z=0) = \phi(z=L_z) = 0 \end{aligned} \right\} \Rightarrow \begin{aligned} \phi(x) &\propto \sin\left(\frac{m\pi}{L_x} x\right) \equiv \sin(k_x x) \\ \phi(y) &\propto \sin\left(\frac{n\pi}{L_y} y\right) \equiv \sin(k_y y) \\ \phi(z) &\propto \sin\left(\frac{p\pi}{L_z} z\right) \equiv \sin(k_z z) \end{aligned} \quad \therefore k_x = \frac{m\pi}{L_x}$$

$m=1, 2, 3, \dots$   
positive integers.

(b) 2nd type of B.C.: Periodic B.C.

$$\left. \begin{aligned} \phi(x=0) = \phi(x=L_x) \\ \phi(y=0) = \phi(y=L_y) \\ \phi(z=0) = \phi(z=L_z) \end{aligned} \right\} \phi(x, y, z) \sim e^{i\left(\frac{m\pi}{L_x} x + \frac{n\pi}{L_y} y + \frac{p\pi}{L_z} z\right)} = e^{i(k_x x + k_y y + k_z z)}$$

$$\therefore k_x = \frac{m'2\pi}{L_x}, \quad m' = \text{integers.}$$

These two types of B.C.'s actually give the same results when we calculate  $\rho_e(E)$ . They are equivalent. It's because:

(a) if  $k_x = \frac{m\pi}{L_x}$ ,  $k_y = \frac{n\pi}{L_y}$ ,  $k_z = \frac{p\pi}{L_z}$  ( $m, n, p = \text{positive integers.}$ )

Each  $(k_x, k_y, k_z)$  state occupies a volume of  $\frac{\pi}{L_x} \cdot \frac{\pi}{L_y} \cdot \frac{\pi}{L_z}$  in  $k$ -space, and we only consider the  $(k_x > 0, k_y > 0, k_z > 0)$  quadrant.

(b) if  $k_x = m' \frac{2\pi}{L_x}$ ,  $k_y = n' \frac{2\pi}{L_y}$ ,  $k_z = p' \frac{2\pi}{L_z}$  ( $m', n', p' = \text{integers}$ )

Each  $(k_x, k_y, k_z)$  state occupies a volume of  $\frac{2\pi}{L_x} \times \frac{2\pi}{L_y} \times \frac{2\pi}{L_z}$  in  $k$ -space, but we have to consider the entire  $k$ -space.

Therefore the results are the same.

### ★ 3D DOS

We use the periodic boundary conditions.

$$\therefore k_x = m \frac{2\pi}{L_x}, \quad k_y = n \frac{2\pi}{L_y}, \quad k_z = l \frac{2\pi}{L_z}, \quad m, n, l \text{ are integers}$$

Each state occupies a volume of  $\left(\frac{2\pi}{L_x}\right) \left(\frac{2\pi}{L_y}\right) \left(\frac{2\pi}{L_z}\right)$  in  $k$ -space.

$$= \frac{(2\pi)^3}{V}$$

$$\therefore \sum_{k_x} \sum_{k_y} \sum_{k_z} = \int \frac{d^3 \vec{k}}{\underbrace{(2\pi)^3/V}_{\text{\# of states in volume } d^3 \vec{k}}}$$

in 3D case, we can replace  $d^3\vec{k}$  by  $4\pi k^2 dk$  then the integration is only w.r.t. a single scalar variable  $k$

$$\therefore \int \frac{d^3\vec{k}}{(2\pi)^3/V} = \int \frac{4\pi k^2 dk}{(2\pi)^3/V} = \int \frac{V}{2\pi^2} k^2 dk \quad \left( = \sum_{k_x} \sum_{k_y} \sum_{k_z} \right)$$

Go back to the very first equation of  $n$

$$n = \frac{2}{V} \sum_{k_x} \sum_{k_y} \sum_{k_z} f_n(E) = \frac{2}{V} \int \frac{V}{2\pi^2} k^2 dk f_n(E) = \int \frac{k^2}{\pi^2} f_n(E) dk$$

We know the relationship between  $E$  &  $k$  is  $E = \frac{\hbar^2 k^2}{2m^*} \Rightarrow \sqrt{\frac{2m^*E}{\hbar^2}} = k$   
 $\therefore dE = \frac{\hbar^2}{m^*} k dk \Rightarrow \frac{m^* dE}{\hbar^2} = k dk$

$$\therefore n = \int \frac{k^2}{\pi^2} f_n(E) dk = \int \frac{f_n(E)}{\pi^2} \frac{\sqrt{2m^*E}}{\hbar} \frac{m^* dE}{\hbar^2} = \int \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E} f_n(E) dE$$

hence this is DOS  $P_e(E)$

★ 2D DOS [In this example, let's use the 1st kind of B.C.'s to practice]  
 i.e.,  $\psi=0$  at the surfaces of a box.

$$\text{still, } n = \frac{2}{V} \sum_{k_x} \sum_{k_y} \sum_{k_z} f_n(E)$$

However, the  $z$  direction is strongly quantized, i.e.  $\Delta k_z = \frac{2\pi}{Lz}$  is a large separation. Therefore, we cannot convert  $\sum_{k_z}$  into integral.

The total energy  $E$  is

$$E = \frac{\hbar^2 k^2}{2m^*} = \frac{\hbar^2 k_x^2}{2m^*} + \frac{\hbar^2 k_y^2}{2m^*} + \frac{\hbar^2 k_z^2}{2m^*} = \frac{\hbar^2 k_{\perp}^2}{2m^*} + \frac{\hbar^2}{2m^*} \left( \frac{l\pi}{Lz} \right)^2$$

$\underbrace{\hspace{10em}}_{\equiv E_{\perp} \text{ (transverse)}} \quad \underbrace{\hspace{5em}}_{\equiv E_z}$

$l = 1, 2, 3, \dots$

$$n = \frac{2}{V} \sum_{k_x} \sum_{k_y} \sum_{k_z} f_n(E) = \frac{2}{V} \sum_{k_x} \sum_{k_y} f_n(E)$$

$$= \frac{2}{V} \sum_{k_x} \left[ \frac{1}{4} \frac{dk_x dk_y}{(\pi/L_x)(\pi/L_y)} f_n(E) \right]$$

each state occupies  
this area in  $k$ -space

→ remember we only consider the 1st quadrant?

$$= \frac{2}{V L_z} \sum_{k_x} \left[ \frac{L_x L_y L_z}{4\pi^2} \int dk_x dk_y f_n(E) \right]$$

$$= \frac{2}{L_z} \sum_{k_x} \left[ \frac{1}{4\pi^2} \int_{k_t=0}^{k_t=\infty} 2\pi k_t dk_t f_n(E) \right]$$

$$L_x L_y L_z = V$$

$$= \frac{2}{L_z} \sum_{k_x} \left[ \frac{1}{2\pi} \int_{E=E_z}^{E=\infty} k_t dk_t f_n(E) \right]$$

<Note>

$$E = \frac{\hbar^2 k_t^2}{2m^*} + E_z$$

$$dE = \frac{\hbar^2}{m^*} k_t dk_t$$

$$= \frac{m^*}{\pi \hbar^2 L_z} \sum_{k_x} \int_{E=E_z}^{E=\infty} f_n(E) dE$$

$$E - E_z = \frac{\hbar^2 k_t^2}{2m^*} \quad \therefore \begin{cases} k_t=0 \Rightarrow E=E_z \\ k_t=\infty \Rightarrow E=\infty \end{cases}$$

Wait, the integration starts from  $E=E_z$ , this is NOT what we want  
(Recall the definition of  $P_e(E)$  :  $n = \int_0^\infty P_e(E) f_n(E) dE$ )

∴ We re-write the above equation as

$$n = \frac{m^*}{\pi \hbar^2 L_z} \sum_{k_x} \int_0^\infty f_n(E) \cdot H(E - E_z) dE \quad \left( \equiv \int_0^\infty P_e(E) f_n(E) dE \right)$$

$$H(E - E_z) = \text{Heaviside function: } \begin{cases} H=0 & \text{when } E < E_z \\ H=1 & \text{when } E \geq E_z \end{cases}$$

∴ Comparing the LHS & RHS of the above equation, we know

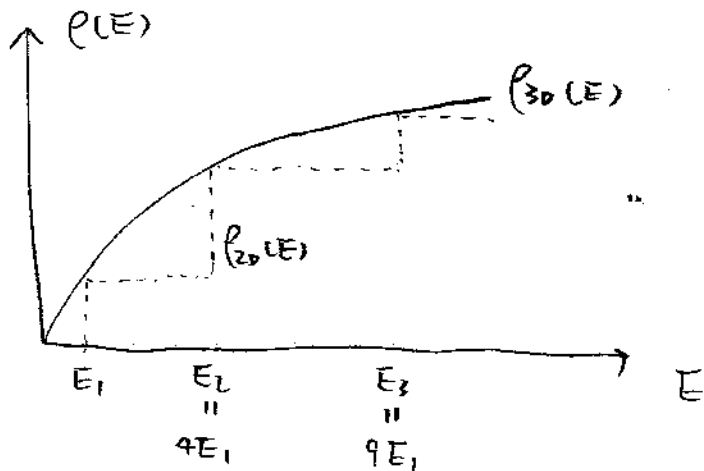
$$\rho_c(E) = \frac{m^*}{\pi \hbar^2 L_z} \sum_l H(E - E_l)$$

for 2D

★ Comparing 3D DOS & 2D DOS

$$\rho_{3D}(E) = \frac{1}{2\pi^2} \left( \frac{2m^*}{\hbar^2} \right)^{3/2} \sqrt{E}$$

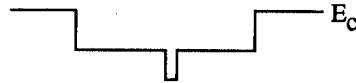
$$\rho_{2D}(E) = \frac{m^*}{\pi \hbar^2 L_z} \sum_l H(E - E_l)$$



# Quantum-Well Lasers

- Workhorse for the semiconductor laser industry.
- Why quantum well?

(a) Single-Quantum-Well Separate-Confinement Heterostructure



(b) Multiple-Quantum-Well Separate-Confinement Heterostructure



(c) Graded-Index Separate-Confinement Heterostructure (GRINSCH)

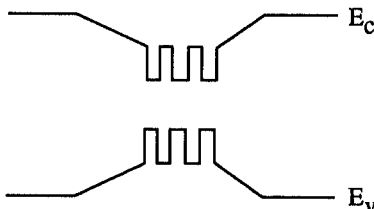


Figure 10.16. Band-gap profiles for (a) single-quantum-well, (b) multiple-quantum-well, and (c) graded-index separate-confinement heterostructure (GRINSCH) semiconductor lasers.

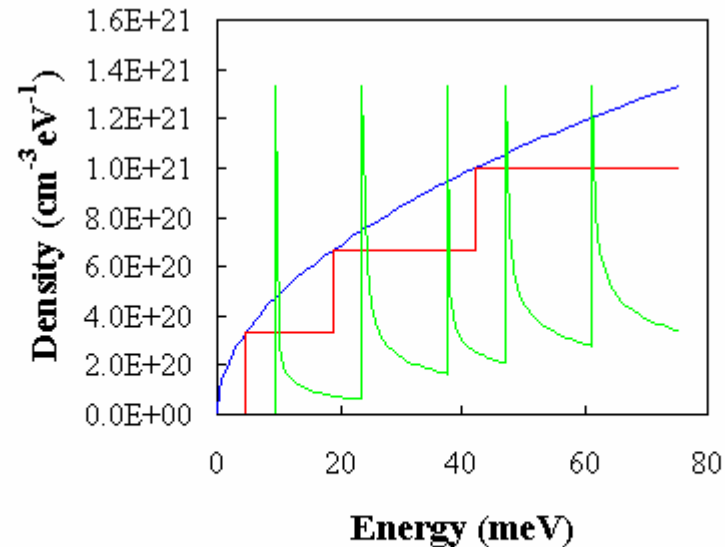
- (1) Tunable wavelength (QW width)
- (2) Smaller threshold current (description see later slides)
- (3) etc...

from: S. L. Chuang –  
Physics of Optoelectronic Devices



# Recall: Density of States

- # of states per unit energy interval per unit volume
- Area bound below is the number of electrons filled up to a certain energy  $E$  (times 2 to include spin)



**Figure 2.4.2:** Density of states per unit volume and energy for a 3-D semiconductor (blue curve), a 10 nm quantum well with infinite barriers (red curve) and a 10 nm by 10 nm quantum wire with infinite barriers (green curve).  $m^*/m_0 = 0.8$ .

[http://ece-www.colorado.edu/~bart/book/book/chapter2/ch2\\_4.htm](http://ece-www.colorado.edu/~bart/book/book/chapter2/ch2_4.htm)



# Absorption

- Absorption curve is proportional to DOS curve (when  $T=0$ )

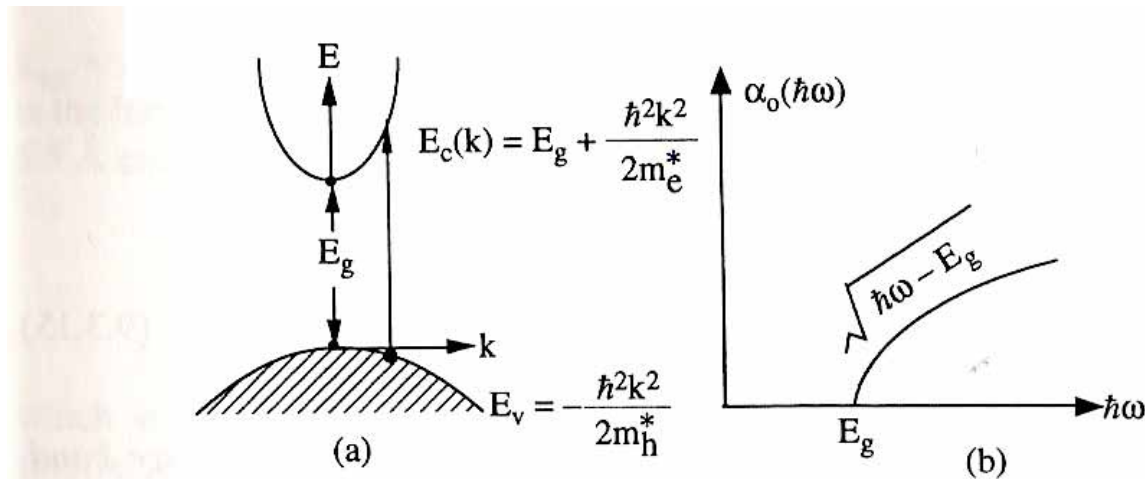


Figure 9.5. (a) Optical absorption in a direct-band-gap semiconductor. (b) The absorption spectrum due to the interband transitions.

from: S. L. Chuang – Physics of Optoelectronic Devices



# Gain

- Population Inversion
- Stimulated Emission
- Gain curve is proportional to DOS curve up to  $F_c - F_v$  along the E axis (when  $T=0$ )

Quasi Fermi energies

Negative absorption = Gain

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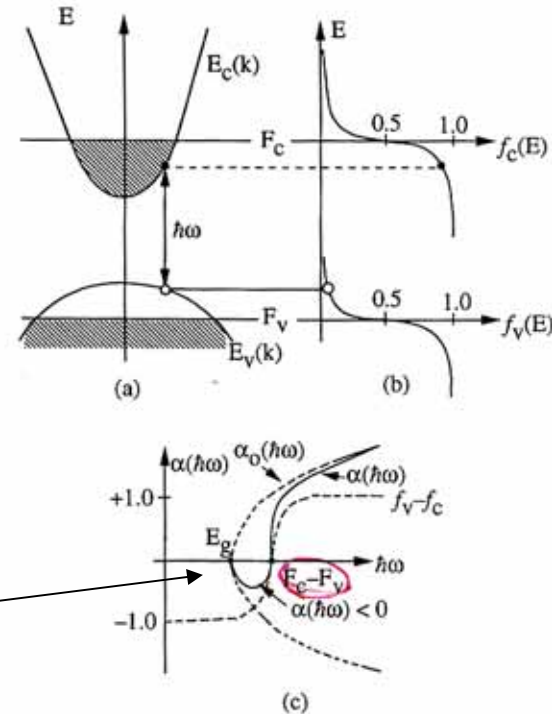
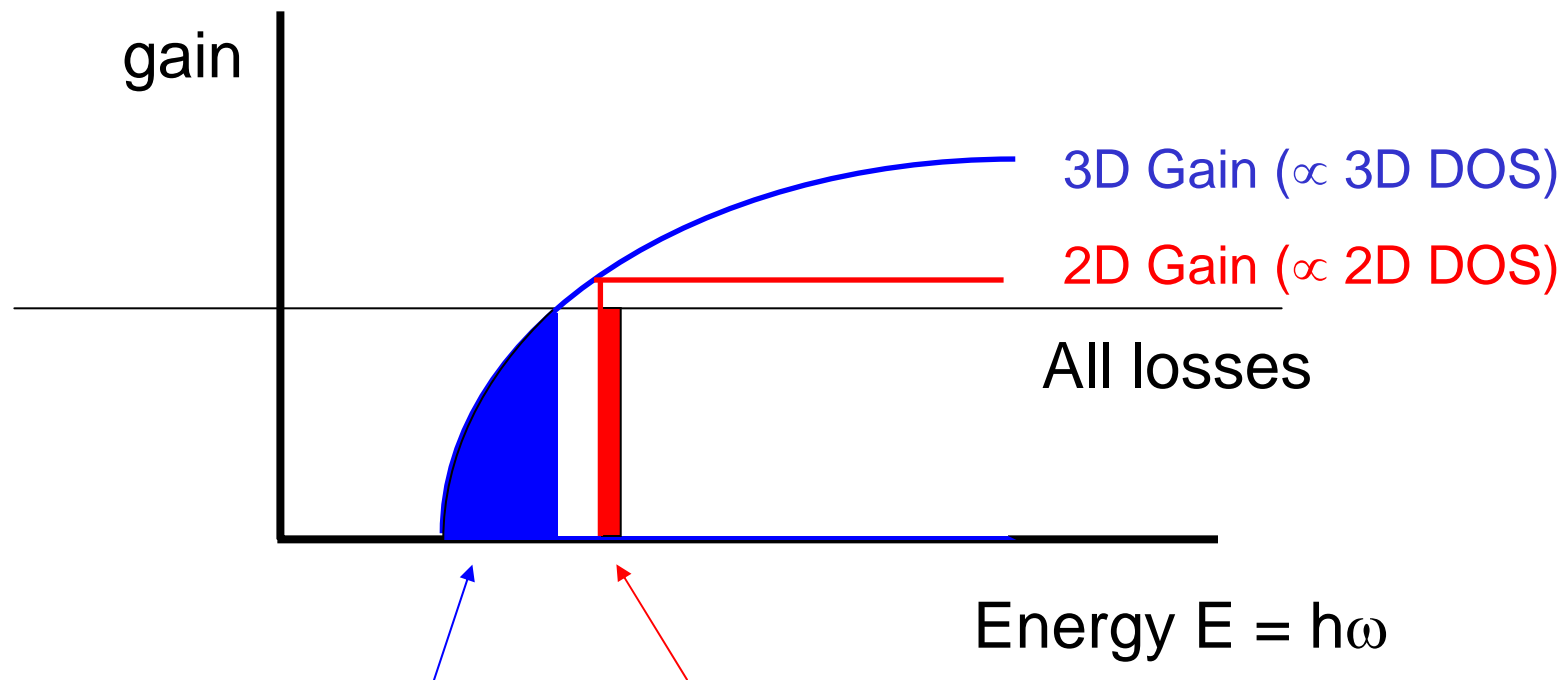


Figure 9.6. (a) Optical transitions between conduction band and valence band. (b) The Fermi-Dirac distributions  $f_c(E)$  and  $f_v(E)$ . (c) The absorption spectrum  $\alpha(h\omega)$ . Note that it is negative for  $E_g < h\omega < F_c - F_v$ , where gain exists.



# Laser Lasing Requirement

- Gain = All the losses in the laser cavity



Lots of carriers required!  
(large threshold current)

Very few carriers required.  
(smaller threshold current)

