

Semiconductor Optoelectronic Devices

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- Perturbation theory and selection rules

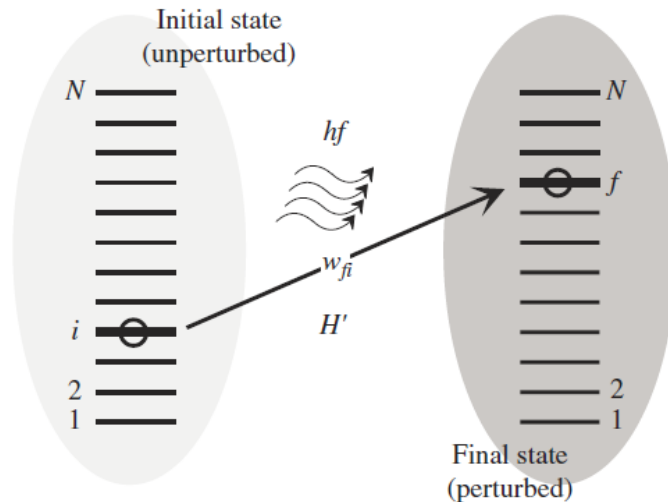


- ❑ In quantum theory, the state of a system subject to **time-independent forces** is described by the solution of the Schrodinger equation, with a given Hamiltonian H_0 , related to the total kinetic and potential energy of electrons and holes.
- ❑ For time-dependent small forces (photons of EM field), its effect can be described by a perturbation of the Hamiltonian (H_0+H'). This is the **perturbation theory**.
- ❑ With the perturbation, the probability of finding a particle in the final state (transited from the initial state) increases **linearly** with time.



Perturbation theory

- Give a certain amount of forces (optical power), the strength of interaction (emitted or absorbed photons per unit time) depends on the magnitude of the **scattering rate**.
- The **scattering rate** is the transition probability from the initial to the final state per unit time (and per unit volume).



Perturbation theory picture of the transition between the initial and final state of a system.



- The perturbation theory shows that the scattering rate w_{fi} is proportional to the magnitude **square of the matrix element M_{fi}** .

$$M_{fi} = \int \psi_f^*(r) H' \psi_i(r) dr$$

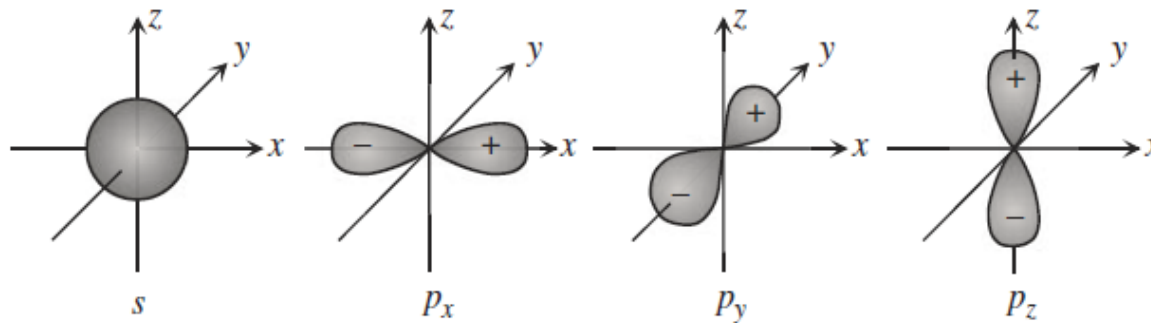
The perturbation Hamiltonian $H' \propto \frac{\partial}{\partial \xi}$

H' and ξ is the direction
of the electric field of the EM wave

- Therefore, the perturbation Hamiltonian can turn an even initial wavefunction to an odd function, and vice versa.



- Near the Gamma point of the FBZ, the conduction band wave function is s-type, while the valence band wavefunction is p-type.



Conduction band (s-type) and valence band (p-type) wavefunctions: probability distribution and wavefunction sign (for p-type).

- The heavy and light hole wave functions is a superposition of p-type wavefunctions:

$$\phi_{HH}(x,y,z) = -\frac{1}{\sqrt{2}}(p_x \pm jp_y)$$

$$\phi_{LH}(x,y,z) = -\frac{1}{\sqrt{6}}(p_x \pm jp_y \mp 2p_z)$$



- Assume the electric field is along x , the initial s -type conduction state and the final p_x state, the corresponding matrix element is non-zero.

Consider, for example, an initial s -type state and a final p_x -state, which is odd along x , even along y and z . The two states can be synthetically described (assume functions are real for simplicity) as

$$s(x, y, z) = e(x)e(y)e(z), \quad p_x(x, y, z) = o(x)e(y)e(z),$$

where e is a (generic) even function, o an odd function of the argument. Assume, for instance, that the perturbation Hamiltonian is $\propto \partial/\partial x$. The application of H' on the initial state leads to an odd function of x ; multiplying by the final p_x state we globally obtain an even function of x (and also of y, z):

$$M_{fi} \propto \int o(x)e(y)e(z) \frac{\partial}{\partial x} [e(x)e(y)e(z)] dx dy dz = \int [o(x)e(y)e(z)]^2 dx dy dz.$$

In this case the kernel is *even*, and $M_{fi} \neq 0$.



- Assume the electric field is along x , the initial s -type conduction state and the final p_y state, the corresponding matrix element is zero.

On the other hand, consider an initial s -type state and a final p_y -state, which is odd along y , even along x and z ; assume again that the perturbation Hamiltonian is $\propto \partial/\partial x$. The application of H' to the initial state leads to an *odd* function of x ; multiplying by the final p_y state, which is *even* along x , we have

$$\begin{aligned} M_{fi} &\propto \int e(x)o(y)e(z) \frac{\partial}{\partial x} [e(x)e(y)e(z)] dx dy dz \\ &= \int e(x)o(y)e(z)o(x)e(y)e(z) dx dy dz \\ &= \underbrace{\int e(x)o(x) dx}_{\text{odd kernel}} \times \underbrace{\int o(y)e(y) dy}_{\text{odd kernel}} \times \underbrace{\int e(z)e(z) dz}_{\text{even kernel}} = 0 \times 0 \times K = 0. \end{aligned}$$

Thus, the integral kernel is an *odd* function of x , an *odd* function of y , and an *even* function of z . In this case, therefore, the integral is zero and $M_{fi} = 0$. Generalizing



- Therefore, given an electric field directed along ξ , the *only interaction possible* is between p_ξ states and s states; for all other p states the matrix element is zero.
- Selection rules is that the initial and final state (wavefunction) pair must have an even-odd or odd-even nature to allow for a transition. Or else, the matrix element is zero, and hence zero interaction strength.
- In bulk semiconductors, the matrix element depends on sets of states (initial or final) of the s and p type. It can be shown that, for any field polarization, there is always some interacting set of initial and final states; **the matrix element is never zero and turns out to be polarization independent**. This also occurs because light and heavy holes are degenerate and therefore contribute in a similar way to the transition.



- ❑ In QW structure, the parity of the initial or final state wavefunctions can be altered by the envelope wavefunction orthogonal to the QW.

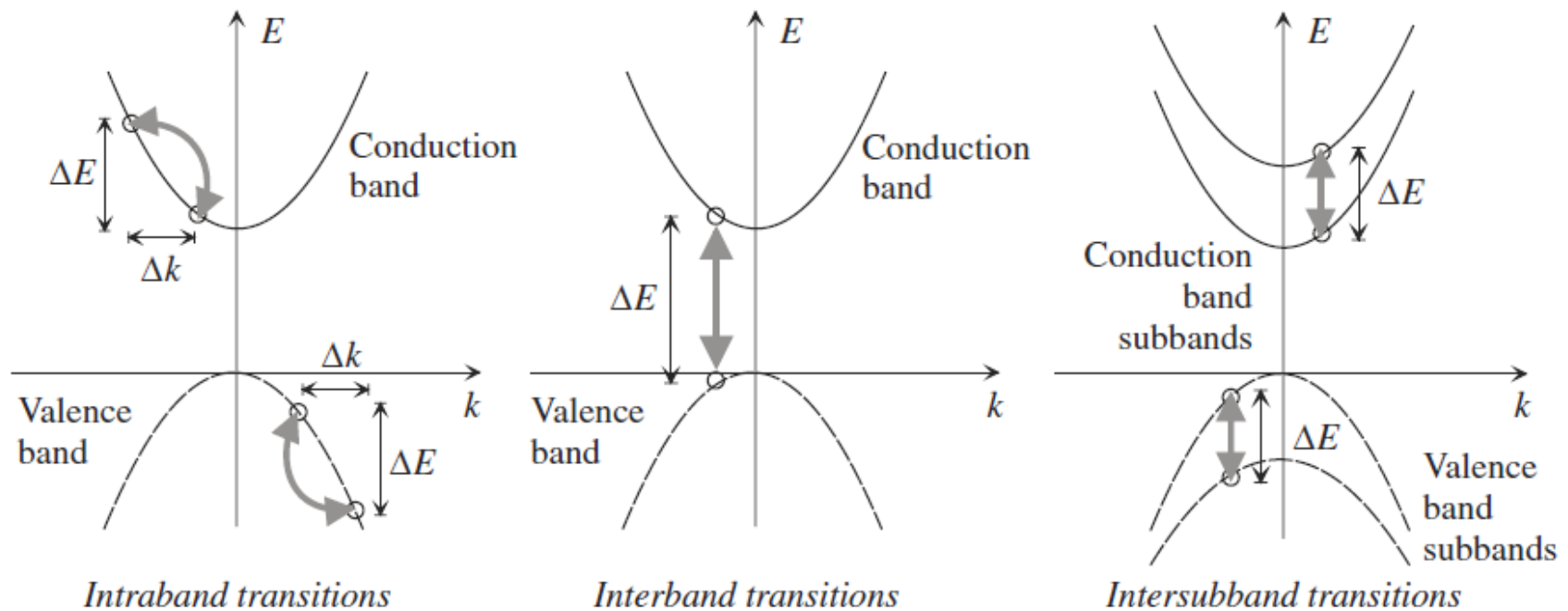
$$\psi(x, y, z) = \exp(-jk_x x) \exp(-jk_y y) \psi(z)$$

$\psi(z)$ is the envelope wavefunction

- ❑ Usually the envelope wavefunction is even in the fundamental state, then alternately odd and even.
- ❑ In addition, in a QW the degeneracy of light holes and heavy holes is removed and the different composition of the corresponding wavefunctions, becomes effective in making **the interaction polarization-dependent**.



- Transitions are classified into intraband transition, interband transition, intersubband transition, and intrasubband transition. Note that intraband and intrasubband transitions are always indirect.



Examples of intraband (left), interband (center), and intersubband (right) transitions.

- The wavefunctions of the QW are given by the envelope wavefunction and the s- or p-like wavefunctions. For the i-th state:

$$\psi_{i,c}(x, y, z) = \psi_i^c(z) s(x, y, z), \quad i=1,2,\dots$$

$$\psi_{i,v\xi}(x, y, z) = \psi_i^v(z) p_\xi(x, y, z), \quad i=1,2,\dots, \quad \xi=x,y,z$$

- The transition matrix element between a p state and a s state is given by

$$\begin{aligned} M_{fi} &\propto \int \phi_{i,c}^* \frac{\partial}{\partial \eta} \phi_{j,v\xi} d\underline{r} = \int \psi_i^{*c}(z) s^*(\underline{r}) \frac{\partial}{\partial \eta} [\psi_j^v(z) p_\xi(\underline{r})] d\underline{r} \\ &= \int \left[\psi_i^{*c}(z) s^*(\underline{r}) p_\xi(\underline{r}) \frac{\partial \psi_j^v(z)}{\partial \eta} + \psi_i^{*c}(z) s^*(\underline{r}) \psi_j^v(z) \frac{\partial p_\xi(\underline{r})}{\partial \eta} \right] d\underline{r} \\ &\approx \int_{-\infty}^{\infty} \psi_i^{*c}(z) \frac{\partial \psi_j^v(z)}{\partial \eta} dz \times \underbrace{\frac{1}{\Omega} \int_{\Omega} s^*(\underline{r}) p_\xi(\underline{r}) d\underline{r}}_{\text{always 0}} + \underbrace{\int_{-\infty}^{\infty} \psi_i^{*c}(z) \psi_j^v(z) dz}_{\neq 0 \text{ if } i,j \text{ are both even/odd}} \\ &\quad \times \underbrace{\frac{1}{\Omega} \int_{\Omega} s^*(\underline{r}) \frac{\partial p_\xi(\underline{r})}{\partial \eta} d\underline{r}}_{\neq 0 \text{ if } \xi=\eta}, \quad i = 1, 2, \dots, \quad \xi, \eta = x, y, z, \end{aligned}$$

□ Therefore, the element matrix is nonzero only when, that is, the transition is possible only when

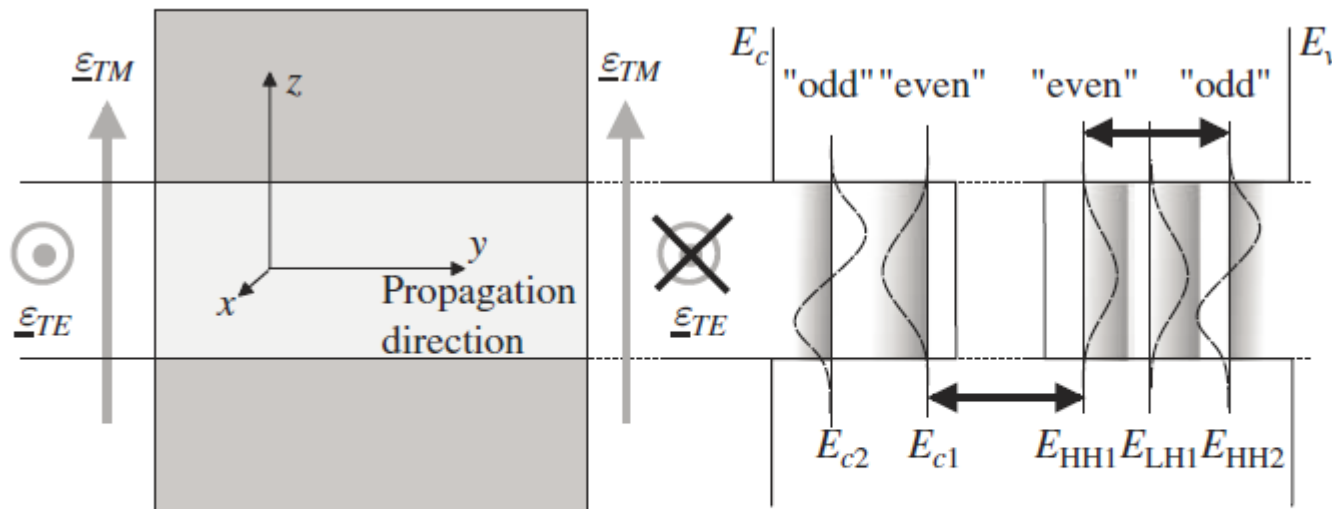
1. The indices of the envelope wavefunctions in the valence and conduction bands are both even or odd (1-1, 2-2, but also in general 1-3, etc.); however, while the 1-1, 2-2 etc. interaction is strong, the 1-3, etc. interaction is typically very weak.
2. The interaction caused by an electric field polarized in the direction ξ involves the valence band state p_{ξ} .



- ❑ In general, if the first condition is met, the interaction will have a different weight according to the field polarization. This happens because, while the LH states include all possible p_x wavefunctions, in the HH states one of these (p_z) does not appear. For HH states, therefore, the matrix element for a z-polarized field is zero, while LH states react (albeit with a different strength) to all polarizations. Since in a QW LH and HH states are not degenerate (and therefore the relevant interactions have a different minimum photon energy), **a global polarization sensitivity of the allowed transitions results.**
- ❑ **The TE polarization (orthogonal to z) causes both LH-C and HH-C transitions, while the TM polarization only causes LH-C transition. The relative transition strength or oscillator strength is**
 - for TE polarization, 3/4 for HH-C, 1/4 for LH-C,
 - for TM polarization, 0 for HH-C, 1 for the LH-C.



- ❑ The allowed transitions for interband are even-even, odd-odd, say, 1-1, 2-2, 1-3. However, strong transitions are typically with equal indices. This is different to the case of bulk semiconductors, which is even-odd.
- ❑ The allowed transitions for intersubband are even-odd as in bulk. However, allowed intersubband transitions usually have low strength.



Examples of selection rules and polarization sensitivity in a QW with the stratification parallel to the z axis (left); the band structure is shown on the right. The thick arrows (right) define allowed interband or intersubband transitions. The horizontal (TE) field is absorbed by the well, the vertical (TM) does not interact.

□ Scattering rates



- The scattering rate is the probability of the transition, or the number of transitions per unit time, between an initial and a final state. The scattering rates for the spontaneous emission, the stimulated emission, and absorption are

$$w_{em}^{sp} = w\delta(E_f - E_i + \hbar\omega)$$

$$w_{em}^{st} = wn_{ph}\delta(E_f - E_i + \hbar\omega)$$

$$w_{abs} = wn_{ph}\delta(E_f - E_i - \hbar\omega),$$

Where w is proportional to the matrix element describing the interaction strength, n_{ph} is the photon number, and delta function indicates that the photon energy has to be the same as the energy difference of states for non-zero scattering rates.



□ For bulk semiconductor,

$$w = \frac{2\pi}{\hbar} \frac{q^2}{m_0^2} \frac{\hbar}{2\omega\epsilon} p_{cv}^2,$$

Where p_{cv} is the **momentum matrix element, or dipole matrix element.**

$$p_{cv} = \int u_{kc}^*(r) p u_{kv}(r) dr$$

u_k is the Bloch wave,

that is, wavefunction at $k=0$ at Γ point

□ The dipole matrix elements of bulk semiconductor according to the polarization are

$$x\text{-polarized light} \rightarrow \begin{cases} \text{HH-C} \rightarrow p_{cv}^2 = \frac{1}{2} p_{cv}^2 \\ \text{LH-C} \rightarrow p_{cv}^2 = \frac{1}{6} p_{cv}^2 \end{cases}$$

$$y\text{-polarized light} \rightarrow \begin{cases} \text{HH-C} \rightarrow p_{cv}^2 = \frac{1}{2} p_{cv}^2 \\ \text{LH-C} \rightarrow p_{cv}^2 = \frac{1}{6} p_{cv}^2 \end{cases}$$

$$z\text{-polarized light} \rightarrow \begin{cases} \text{HH-C} \rightarrow p_{cv}^2 = 0 \\ \text{LH-C} \rightarrow p_{cv}^2 = \frac{2}{3} p_{cv}^2 \end{cases}$$



- In bulk semiconductors, HH and LH are degenerate. For unpolarized light, the total average momentum matrix element for the valence band is $2p_{cv}^2/3$, thus, the average momentum matrix element for HH and LH is the same $p_{cv}^2/3$.
- Therefore, the rate for unpolarized light interacting with a bulk semiconductor is

$$w = \frac{2\pi}{\hbar} \frac{q^2}{m_0^2} \frac{\hbar}{2\omega\epsilon} \frac{2}{3} p_{cv}^2 \quad \text{J m}^3 \text{ s}^{-1}.$$

- In addition, the scattering rate has to take into account the **joint density of states**, and the state occupation probability that **the initial state is filled while the final state is empty because of the exclusion principle**.

$$N_{cv}(\hbar\omega) = \frac{(2m_r^*)^{3/2}}{2\pi^2\hbar^3} \sqrt{\hbar\omega - E_g} \quad \text{m}^{-3}\text{J}^{-1}.$$



- Then, the absorption scattering rate is given by

$$\mathcal{W}_{abs}(\hbar\omega) = \omega n_{ph} N_{cv}(\hbar\omega) [1 - f_h(E_i(\hbar\omega))] [1 - f_n(E_f(\hbar\omega))] \text{ s}^{-1}.$$

- The total emission scattering rate is given by

$$\begin{aligned} \mathcal{W}_{em}(\hbar\omega) &= \mathcal{W}_{em}^{SP}(\hbar\omega) + \mathcal{W}_{em}^{st}(\hbar\omega) \\ &= \omega(1 + n_{ph}) N_{cv}(\hbar\omega) f_n(E_n(\hbar\omega)) f_h(E_h(\hbar\omega)) \text{ s}^{-1}. \end{aligned}$$

- The rate of stimulated emission and of spontaneous emission relation is

$$\mathcal{W}_{em}^{st} = n_{ph} \mathcal{W}_{em}^{SP}.$$

Example 2.3



□ The EM wave standpoint

---absorption and gain



- From the EM wave standpoint, the interaction of EM wave and the semiconductor is characterized by the complex dielectric permittivity or the complex propagation constant.
- From the semiconductor standpoint, the interaction is characterized by the radiative recombination rate and generation rate.
- From the EM wave standpoint, the photon density change is given by

$$\rho_{ph}(x) = \rho_{ph}(0) \exp(-\alpha x)$$

α is the absorption coefficient,

which can be positive or negative

- The macroscopic photon density is linked with the microscopic scattering rates (per unit volume) as

$$\frac{d}{dt} \rho_{ph}(t) = \frac{c_0}{n_r} \frac{d}{dx} \rho_{ph}(x)$$

$$= W_{st} - W_{abs}$$

$$= w \rho_{ph} N_{cv} f_h(E_h) f_n(E_n) - w \rho_{ph} N_{cv} [1 - f_h(E_h)][1 - f_n(E_n)]$$

where spontaneous emission is neglected



- From the above two relations, we can get the expression of the absorption coefficient,

$$\begin{aligned}\alpha &= \frac{n_r}{c_0} w N_{cv} \left\{ [1 - f_h(E_h)][1 - f_n(E_n)] - f_h(E_h)f_n(E_n) \right\} \\ &= \frac{n_r}{c_0} w N_{cv} [1 - f_h(E_h) - f_n(E_n)]\end{aligned}$$

- If the absorption coefficient is negative, we say the semiconductor has a **gain**, and the **gain coefficient** is given by

$$g = -\alpha = \frac{n_r}{c_0} w N_{cv} [f_h(E_h) + f_n(E_n) - 1]$$

- Under thermal equilibrium condition, f_h and f_n is small and close to zero. So the semiconductor has positive absorption coefficient, and can absorb photons.
- Under carrier injection, electrons are excited to the conduction band, f_h and f_n becomes large, can be close to one. So the semiconductor has positive gain coefficient, and can emit photons with stimulated emission.



- In order to have a positive gain, the occupation probability must

$$f_h(E_h) + f_n(E_n) - 1 > 0$$

or

$$f_n(E_n) - f_n(E_h) > 0$$

- That is,

$$\frac{1}{1 + \exp\left(\frac{E_n - E_{Fn}}{k_B T}\right)} + \frac{1}{1 + \exp\left(-\frac{E_h - E_{Fh}}{k_B T}\right)} - 1 > 0$$

- Thus,

$$E_{Fn} - E_{Fh} > E_n - E_h \geq E_g$$

- In this **population inversion condition**, $n_p \gg n_i^2$, this only happens in a forward biased pn junction or heterojunction. Conversely, in a depleted region, $n_p \ll n_i^2$ and therefore absorb photons.



- ❑ Assume the Fermi distribution is at 0 K as a step function, that is, f is either 0 or 1.
- ❑ Assume the active region is lightly doped, that is, $n \sim p$.
- ❑ For $E_{ph} < E_g$, the joint density of state is always zero, and always $g=0$, whatever the carrier population is.
- ❑ For $E_{ph} > E_g$, if the population $n < n_{ivc}$, that is, $E_{fn} - E_{fh} < E_g$. Then,

$f_n \sim f_h \sim 0$ for all photon energies

$$g = -\alpha = \frac{n_r}{c_0} w N_{cv} [f_h(E_h) + f_n(E_n) - 1] = -\frac{n_r}{c_0} w N_{cv}$$

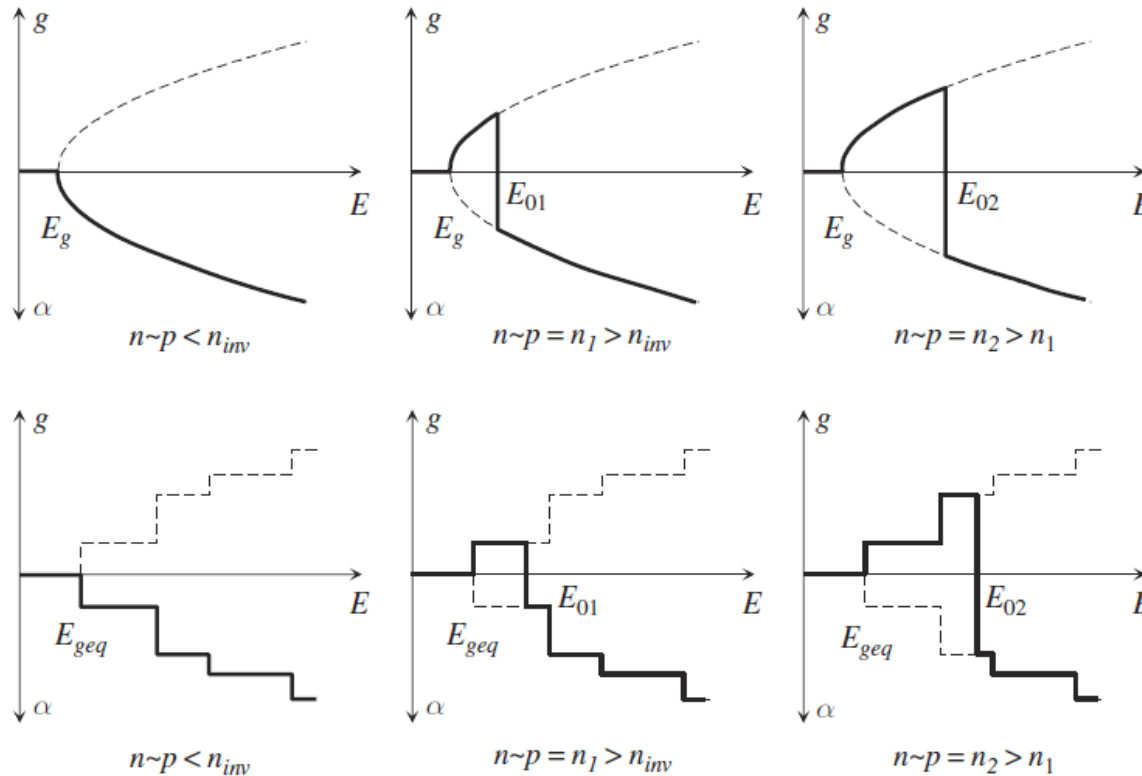
- ❑ For $E_{ph} > E_g$, if the population $n > n_{ivc}$, that is, $E_{fn} - E_{fh} > E_g$. Then,

$f_n \sim f_h \sim 1$ for $E_{ph} < E_{fn} - E_{fh}$; $f_n \sim f_h \sim 0$ for $E_{ph} > E_{fn} - E_{fh}$;

$$g = \begin{cases} = \frac{n_r}{c_0} w N_{cv}, & \text{for } E_{ph} < E_{fn} - E_{fh} \\ = -\frac{n_r}{c_0} w N_{cv}, & \text{for } E_{ph} > E_{fn} - E_{fh} \end{cases}$$



Therefore, the gain profile is linearly proportional to the joint density of states.



Qualitative behavior of gain at $T = 0$ K as a function of the photon energy from below inversion (left) and for increasing injected carrier density above inversion (center and right). Above: bulk (3D); below: QW (2D) with staircase joint density of states.



□ For temperatures above 0 K, the gain profile vs. energy can be obtained from the following procedure:

1. From $n \sim p$, determine the electron and hole quasi-Fermi levels through the Joyce-Dixon formula

$$E_{fn} = E_c + k_B T \left[\log \frac{n}{N_c} + \frac{1}{\sqrt{8}} \frac{n}{N_c} \right];$$

$$E_{fp} = E_v - k_B T \left[\log \frac{p}{N_v} + \frac{1}{\sqrt{8}} \frac{p}{N_v} \right];$$

2. From the photon energy, determine the initial and the final electron energy

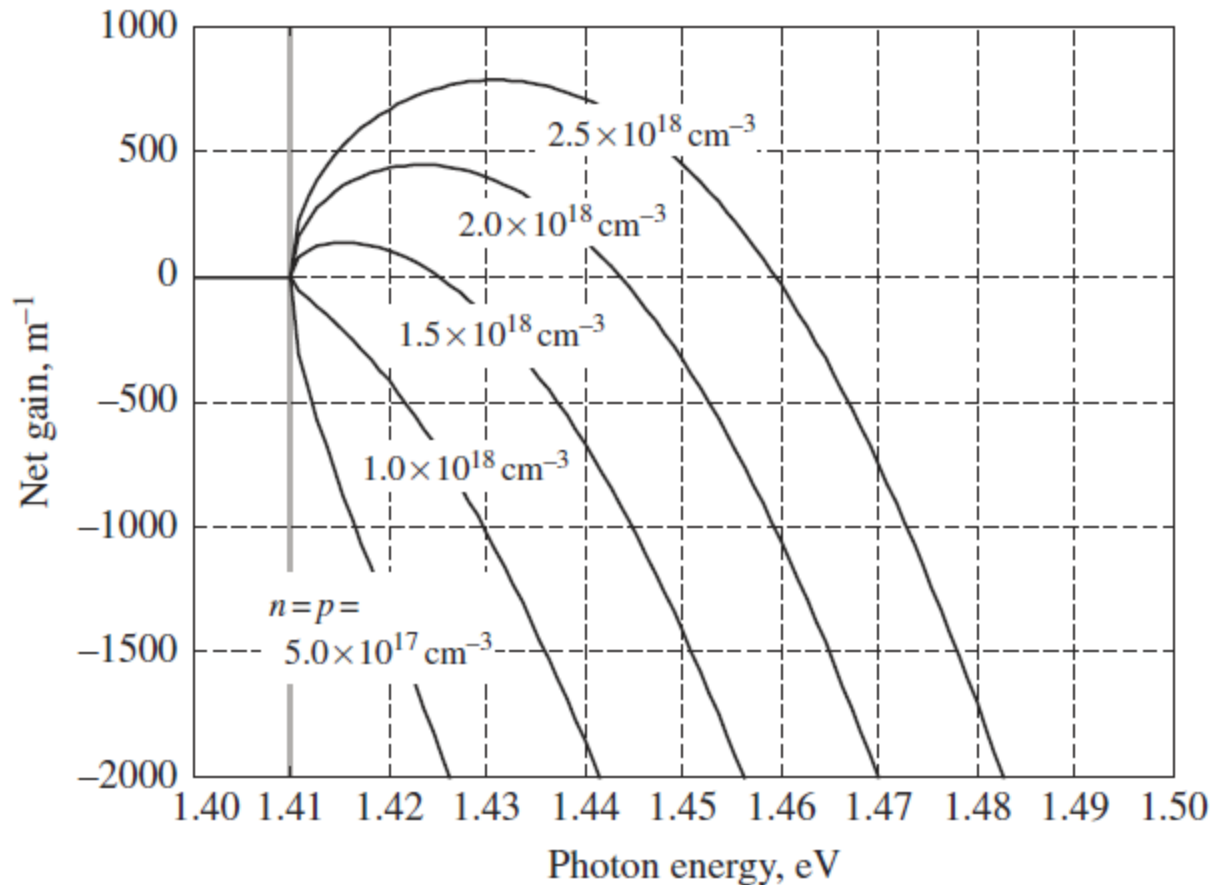
$$E_i = E_v - \frac{m_r^*}{m_h^*} (\hbar\omega - E_g)$$

$$E_f = E_c + \frac{m_r^*}{m_n^*} (\hbar\omega - E_g)$$

3. Finally, determine the occupation probability through the quasi-Fermi distribution and obtain the gain

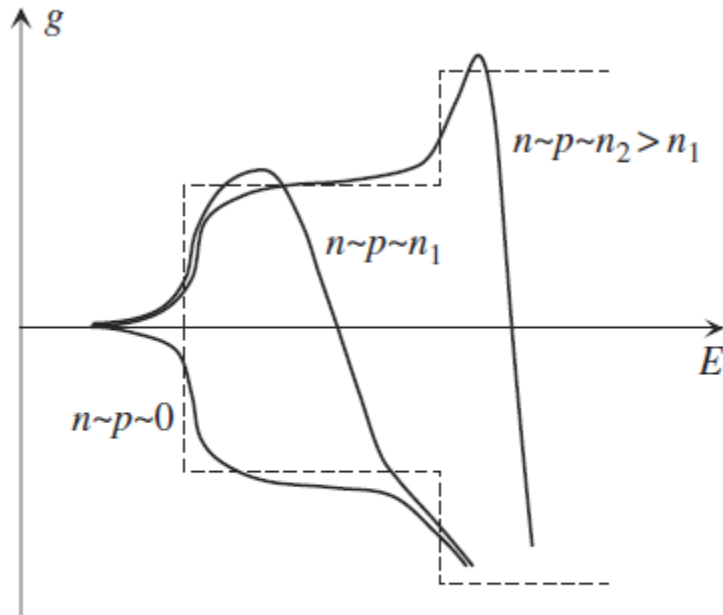


Gain profile of double heterojunction



Gain profile in a AlGaAs/GaAs double heterojunction as a function of the electron and hole injected populations.





Qualitative behavior of the gain of a QW for different injected population density, starting from depletion conditions.



- ❑ For laser diodes at high injection condition, the carrier lifetime of stimulated emission is in the picosecond range. For the lasing photon energy, carriers in the corresponding E_n & E_f deplete very fast. The main mechanism for supplying carriers to both states are phonon scattering, whose characteristic time constant is around 1 ps, which is not fast enough to compensate the carrier depletion in and around E_n & E_f , and thus to maintain the quasi-Fermi distribution. This effect is called **spectral hole burning**.
- ❑ Because the spectral hole burning, the occupation probability f_n and f_h decrease, and so does the gain. This effect is called **gain compression**.

$$g = \frac{g_F}{1 + \xi \rho_{ph}}$$

g_F is the unperturbed (quasi-Fermi) gain

ξ is the gain compression factor

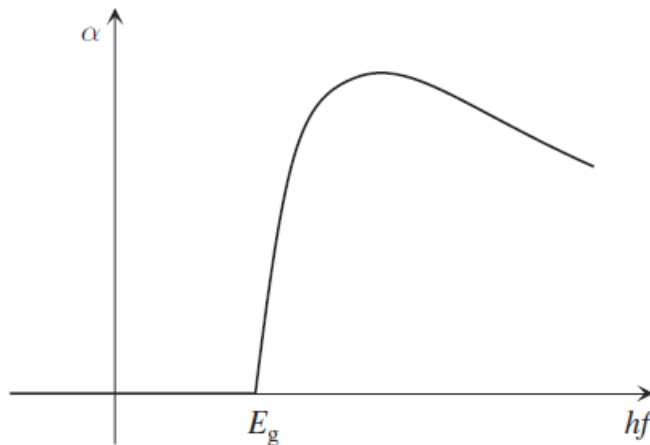
- ❑ Gain compression limits the stimulated carrier lifetime, and therefore the laser dynamics.



- For a depleted region (reverse bias), $f_n \sim f_h \sim 0$. The absorption coefficient for direct-bandgap bulk semiconductors is

$$\alpha = \frac{n_r}{c_0} w N_{cv}(\hbar\omega) = \frac{\pi q^2 \hbar n_r}{2\epsilon m_0 c_0} \frac{2}{3} \left(\frac{2p_{cv}^2}{m_0} \right) \frac{1}{\hbar\omega} N_{cv}(\hbar\omega)$$

$$\alpha = \frac{q^2 n_r (2m_r^*)^{3/2}}{2\pi \epsilon \hbar^2 m_0 c_0} \frac{2}{3} \left(\frac{2p_{cv}^2}{m_0} \right) \frac{1}{\hbar\omega} \sqrt{\hbar\omega - E_g} \approx \frac{K}{\hbar\omega} \sqrt{\hbar\omega - E_g},$$

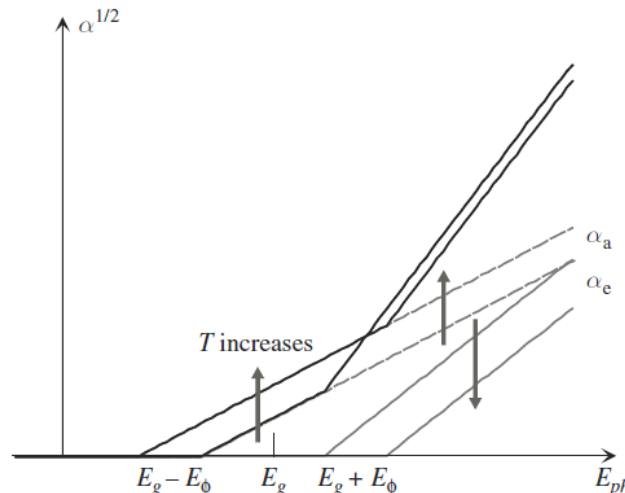


Theoretical behavior of the absorption coefficient in a direct-bandgap semiconductor.

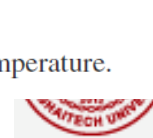
- For indirect-bandgap semiconductor, the photon absorption requires the help of phonon emission and phonon absorption. So the absorption coefficient is

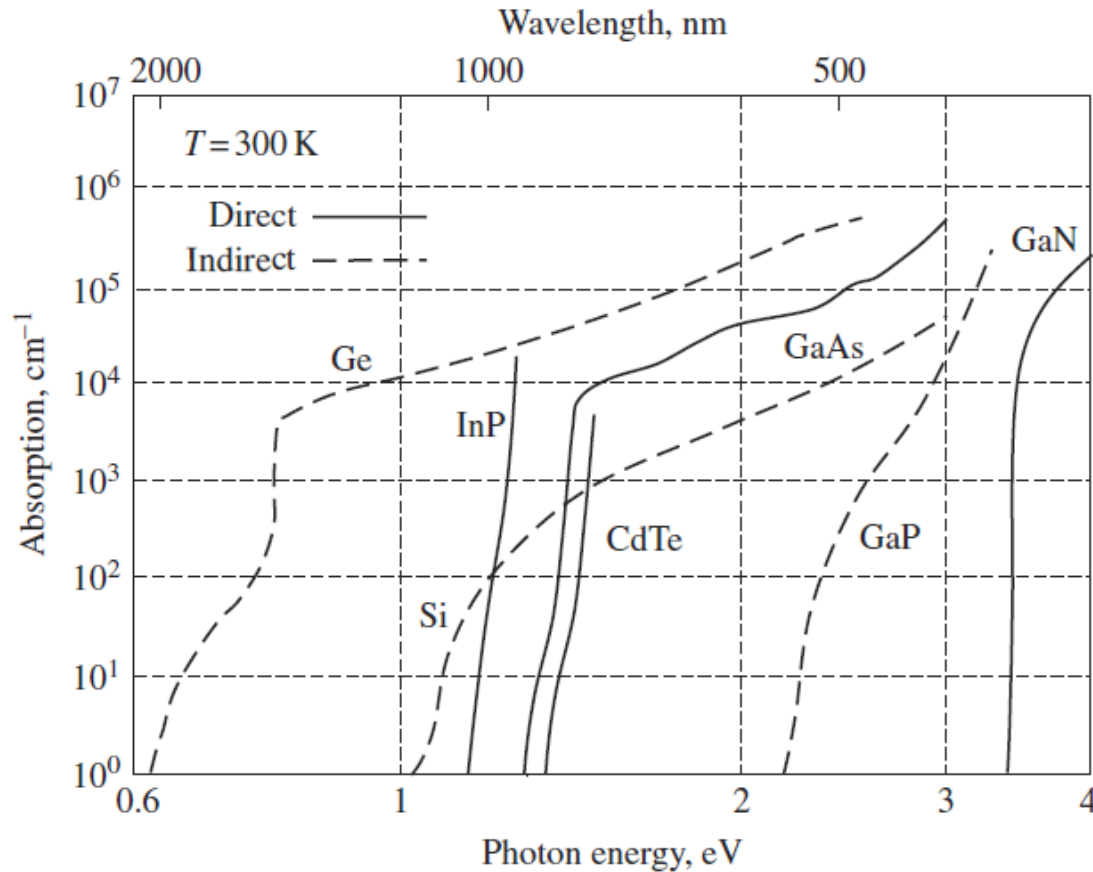
$$\alpha = \alpha_e + \alpha_a$$
$$\alpha_e \propto (\hbar\omega - E_g - E_\phi)^2, \quad \hbar\omega > E_g + E_\phi$$
$$\alpha_a \propto (\hbar\omega - E_g + E_\phi)^2, \quad \hbar\omega > E_g - E_\phi.$$

- Note that the phonon energy increases with the temperature.
- Note that the absorption edge can be smaller than the bandgap energy, different to indirect bandgap semiconductors.



Absorption coefficient of an indirect-bandgap semiconductor at different temperature.

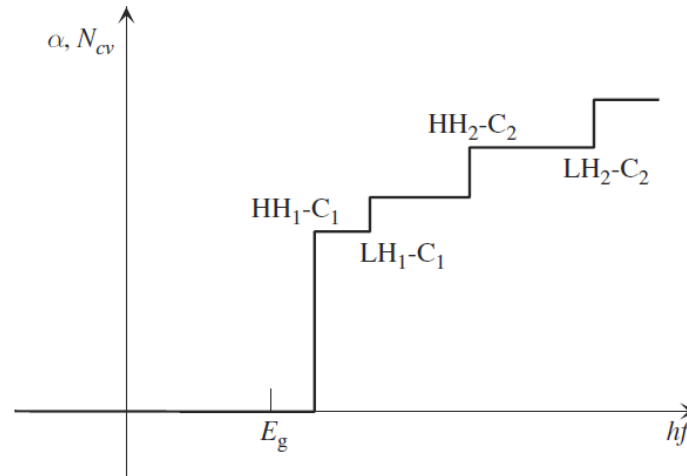
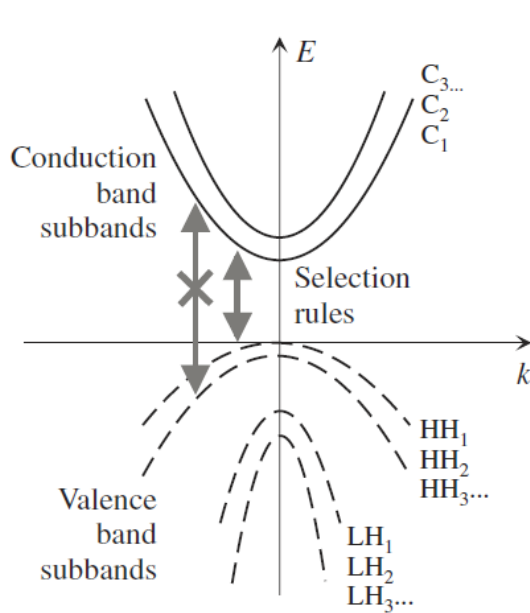




Absorption profile of some direct- and indirect-bandgap semiconductors (adapted from [1]).



- In a QW, conduction and valence subbands exist. The conduction subbands are $C_1, C_2, C_3\dots$, and the valence subbands are $HH_1, LH_1, HH_2, LH_2, HH_3, LH_3\dots$



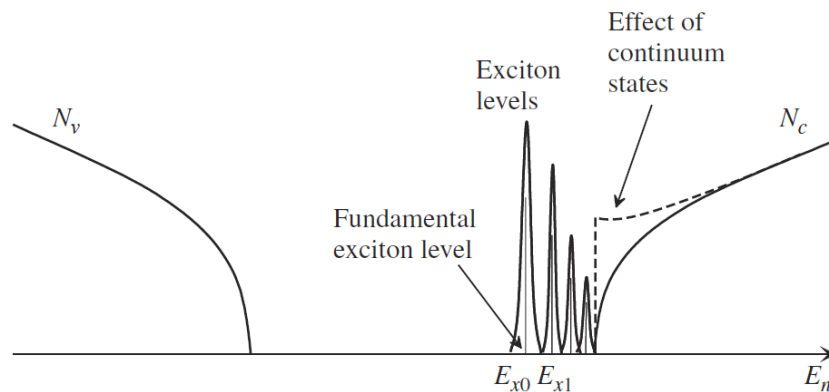
Absorption profile (neglecting exciton peaks) and joint density of states for a QW: staircase behavior with steps corresponding to the allowed transitions.

Dispersion relation for a QW with a qualitative picture of the HH and LH bands.

- The ideal absorption profile is similar to the staircase behavior of the QW JDOS, but only the steps relative to allowed transitions having non-negligible strength are present.



- ❑ However, the practical absorption profile shows sharp resonance peaks close to the bandgap energy due to the **excitons**.
- ❑ An **exciton** is a weakly bound state (束缚态) of an electron and a hole which are attracted to each other by the Coulomb force. The binding energy is small, usually less than 10 meV in bulk semiconductors. This weak bound e-h pairs only appear at low temperature, while break at room temperature, where the average energy of carriers is on the order of 40 meV. However, QW can have excitons even at room temperature due to the much larger binding energy.
- ❑ Excitons can introduce a set of closely packed discrete levels in the forbidden band of semiconductors, plus an additional continuum set of state that merge with the conduction band state density.



Qualitative picture of exciton levels in the semiconductor density of states.



- The position of the exciton levels can be explained from the fact that a small amount of energy breaks the exciton, bringing the bound electron into the conduction band. The exciton level can therefore be understood as an energy level immediately below the conduction band, in much the same way as a shallow donor level is located immediately below the conduction band edge. In such conditions, an ionization energy of the order of 10 meV is enough to promote an electron trapped in the shallow level into the conduction band.
- The E-k relation of excitons is given by

$$E_{nx}(\underline{k}_x) = E_g - \frac{R_\infty^*}{n^2} + \frac{\hbar^2 \underline{k}_x^2}{2m_x^*}, \quad n = 1, 2, \dots, \infty,$$

$$R_\infty^* = \frac{m_r^*}{m_0} \frac{1}{n_r^4} R_\infty,$$

where the exciton effective mass and the Rydberg constant are

$$m_x^* = m_h^* + m_n^*$$

$$R_\infty = 13.605 \text{ eV}$$

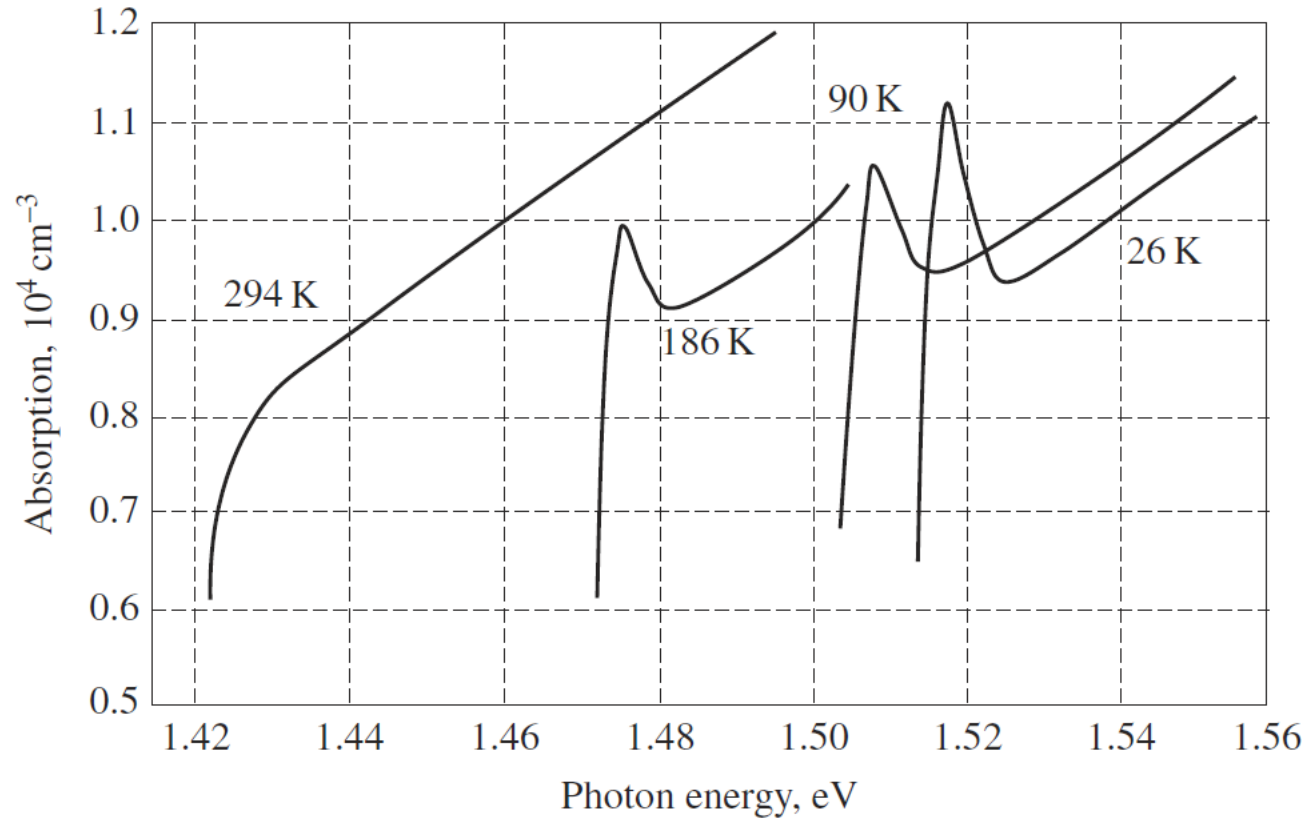
Example 2.4



- ❑ Excitons can interact with photons having energies immediately below the absorption edge E_g , thus creating strong absorption peaks and an increase of the absorption profile for $E_{ph} \approx E_g$. Such peaks appear close to the absorption edge energy in bulk semiconductors or close to each staircase step in the QW response, and merge with the step due to the effect of finite linewidth.
- ❑ In a bulk material like GaAs, exciton peaks disappear at ambient temperature and are only visible at low T . In a quantum well, however, the binding energy of excitons is substantially larger; in fact, it can be shown that, in this case, the **binding energy** of the fundamental exciton state is four times larger than in bulk semiconductors.

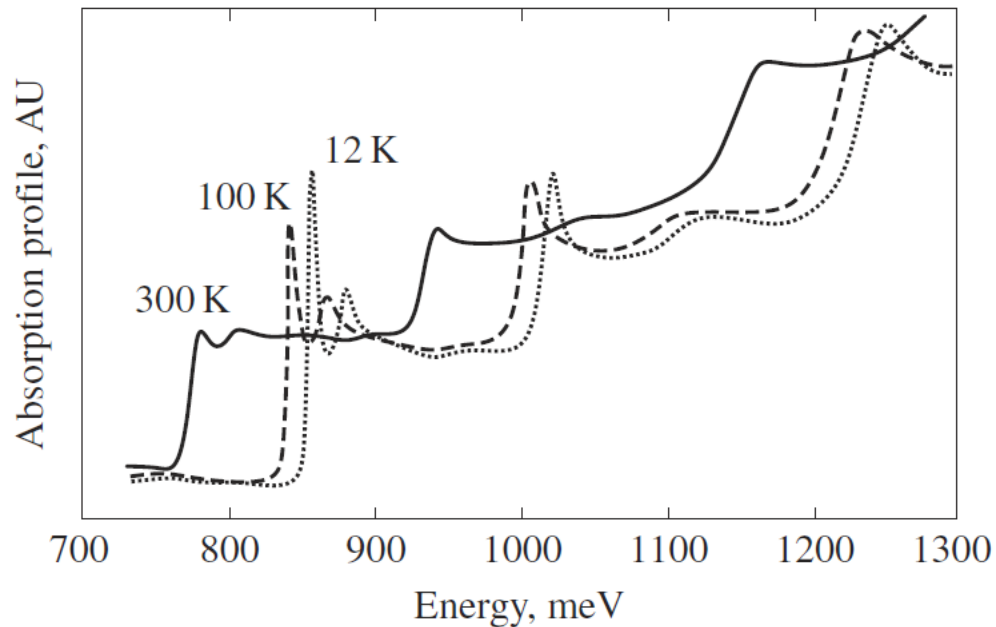
$$E_x = E_{g,\text{eff}} - E_{1x}(0) = \frac{4m_r^*}{m_0} \frac{1}{n_r^4} R_\infty.$$





Absorption profiles in bulk GaAs vs. temperature, showing the effect of excitons. From [15], Fig. 3, (©1962 American Physical Society).





Measured absorption profile of InGaAs/InAlAs 10nm/200m undoped MQW. The exciton peaks are clearly visible also at ambient temperature. From [16] Fig. 2 (a) (©1988 IEEE).

