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WINTER COLLEGE ON
LASER PHYSICS: SEMICONDUCTOR LASERS
AND INTEGRATED OPTICS

(22 February - 11 March 1988)

STIMULATED EMISSION IN SEMICONDUCTORS

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RELATIONSHIPS BETWEEN ABSORPTION, STIMULATED EMISSION, AND SPONTANEOUS EMISSION

Introductory Remarks

The simplest description of the interaction of light and free-carrier electrons in a semiconductor is based on the Einstein relations, which connect the rates of absorption, stimulated emission, and spontaneous emission. Although the Einstein relations were originally expressed for an atomic system in free space with two sharp energy levels, these relations have been generalized to broad-band spectra and are useful for semiconductors with a distribution of states in the valence and conduction bands. With this approach, the blackbody radiation is considered to be the radiation field. Use will also be made of the blackbody radiation in relating the emission that results from external excitation to the measured absorption spectrum. The photon and energy density distributions for blackbody radiation are derived below and then utilized in the relationships between absorption, stimulated emission, and spontaneous emission.

Blackbody Radiation

Blackbody radiation is the equilibrium emission within a cavity at a uniform temperature and is of interest because of its relationship to various nonequilibrium absorption and emission processes. Very thorough discussions of blackbody radiation have been given in numerous texts, and a descriptive treatment is given by Kestin and Dorfman. The quantities to be derived for blackbody radiation are the number of photons per unit

volume and unit frequency and the number of photons per unit volume and unit energy, which are the photon density distributions. Two quantities are necessary to express the photon density distribution. One is the density of states or the number of allowed solutions (modes or states) as obtained from Maxwell's equations. The other is the probability that a photon will occupy that state and is the Bose–Einstein distribution law.

Consider a cubic enclosure with dimension L and assume that the allowed solutions of the wave equation are independent of the boundary conditions as long as all dimensions of the enclosure are very large compared to the wavelengths being considered. Although difficult to prove, this assumption is generally accepted, and a simple demonstration of independence has been given by Joyce. The simplest boundary conditions are periodic and require the minimum sample dimension to be many wavelengths. In Chapter 2, the one-dimensional wave equation (with β replaced by k_x) was given as

$$(\partial^2 \mathcal{E}_x/\partial z^2) + k_x^2 \mathcal{E}_x = 0, \qquad (2.2\text{-}25)$$

where

$$k_x = 2\pi/\lambda \qquad (2.2\text{-}30)$$

and k_x is designated as the propagation constant or wave vector. The wave traveling in the $+z$ direction was written as

$$\mathcal{E}_x(z, t) = A\cos(\omega t - k_x z). \qquad (2.2\text{-}27)$$

The periodic boundary condition requires that

$$\mathcal{E}_x(0, t) = \mathcal{E}_x(L, t) \qquad (3.2\text{-}1)$$

which restricts k_x to the discrete values of

$$k_x = 2\pi m_x / L, \qquad (3.2\text{-}2)$$

where m_x is an integer $(0, \pm 1, \pm 2, \pm 3, \ldots)$.

For the cubic enclosure, the three-dimensional wave equation [Eq. (2.4-8)] with periodic boundary conditions extends the one-dimensional case to the restriction

$$k_x = 2\pi m_x/L, \qquad k_y = 2\pi m_y/L, \qquad k_z = 2\pi m_z/L, \qquad (3.2\text{-}3)$$

where m_x, m_y, m_z are integers $(0, \pm 1, \pm 2, \pm 3, \ldots)$. These discrete values of k_x, k_y, and k_z give discrete values of $\mathcal{E}$ which are called "modes." The particlelike nature of electromagnetic radiation is represented by photons with energy

$$E = h\nu = |\mathbf{p}|c, \qquad (3.2\text{-}4)$$

and momentum **p** with the components

$$p_x = \hbar k_x, \qquad p_y = \hbar k_y, \qquad p_z = \hbar k_z, \tag{3.2-5}$$

where h is Planck's constant and $\hbar$ is $h/2\pi$. The discrete values of k_x, k_y, and k_z give discrete photon energies, and therefore the allowed solutions are also referred to as "states." The problem now becomes one of counting the number of these states and deriving expressions for their number per unit volume, which is the density of states. The density of states determination is encountered in several areas of physics (see, for example, Mandl[16]).

The density of states is derived in terms of the wave vector **k**, and therefore it is useful to introduce the concept of **k** space with

$$\mathbf{k} = \mathbf{a}_x k_x + \mathbf{a}_y k_y + \mathbf{a}_z k_z, \tag{3.2-6}$$

where $\mathbf{a}_x$, $\mathbf{a}_y$, and $\mathbf{a}_z$ are unit vectors in the x, y, and z directions. The wave vector **k** in terms of k_x, k_y, and k_z given by Eq. (3.2-3) is shown in Fig. 3.2-1. The unit volume in **k**-space is indicated by the dotted cube in Fig. 3.2-1 and has a volume given by

$$\text{unit volume in } \mathbf{k}\text{-space} = (2\pi/L)^3. \tag{3.2-7}$$

Only the values of **k** given by Eq. (3.2-3) are allowed, and it can then be concluded that the number of allowed values of **k** in any volume V_k in **k**-space is the number of cubes of side $2\pi/L$ in that volume.

The density of states may be found from the number of states in **k**-space between **k** and $(\mathbf{k} + d\mathbf{k})$. Let the volume of a thin spherical shell be $4\pi k^2\,dk$. The unit density in **k**-space is the reciprocal of the unit volume given in Eq. (3.2-7). Then the number of states in **k**-space is the volume times the density which is

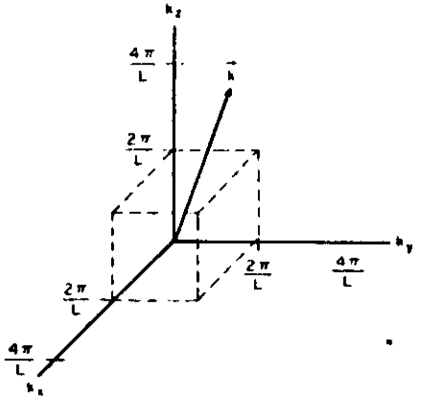


FIG. 3.2-1 A plot of k-space in terms of k_x, k_y, and k_z given by Eq. (3.2-3) for periodic boundary conditions.

$$dN(k) = 2(L/2\pi)^3 4\pi k^2\,dk, \tag{3.2-8}$$

where the factor of 2 accounts for two different states of polarization for a photon of a given momentum. In Chapter 2, these polarizations were designated as transverse electric (TE) and transverse magnetic (TM). The density of states is the number of states per unit volume of the solid $V = L^3$ and is

$$dN(k) = (k^2/\pi^2)\,dk. \tag{3.2-9}$$

For a dielectric solid, the wave vector is

$$k = 2\pi/\lambda = (2\pi/c)\bar{n}\nu, \tag{3.2-10}$$

where $\bar{n}$ is the refractive index and ν is the frequency. Then,

$$dk = 2\pi(\bar{n}/c)\,d\nu\,[1 + (\nu/\bar{n})(d\bar{n}/d\nu)], \tag{3.2-11}$$

where the term in the brackets is the refractive index dispersion and is unity for free space. Equation (3.2-9) becomes

$$dN(\nu) = (8\pi\bar{n}^3\nu^2/c^3)[1 + (\nu/\bar{n})(d\bar{n}/d\nu)]\,d\nu. \tag{3.2-12}$$

The average number of photons per state $\langle n_i \rangle$ is given by the Bose–Einstein distribution law, which applies to a system of identical particles that are indistinguishable and have integral spin:[17]

$$\langle n_i \rangle = [\exp(h\nu_i/kT) - 1]^{-1}. \tag{3.2-13}$$

Therefore, the photon density distribution $dD(\nu)$ is given by $\langle n_i \rangle\,dN(\nu)$, which is

$$dD(\nu) = \frac{8\pi\bar{n}^3\nu^2}{c^3}\,\frac{1 + (\nu/\bar{n})(d\bar{n}/d\nu)}{\exp(h\nu/kT) - 1}\,d\nu. \tag{3.2-14}$$

Often the blackbody photon density distribution is given as the energy distribution, which is the photon energy $h\nu$ times the photon density distribution $dD(\nu)$. Equation (3.2-14) gives the photon density distribution in units of the number of photons per unit volume. For the analysis that follows, it is more convenient to express the photon density distribution as the number of photons per unit volume and unit energy, so that from Eq. (3.2-4) $d\nu = dE/h$, and

$$dD(E) = \frac{8\pi\bar{n}^3E^2}{h^3c^3}\,\frac{1 + (E/\bar{n})(d\bar{n}/dE)}{\exp(E/kT) - 1}\,dE. \tag{3.2-15}$$

Then, the spectral density at a specific energy E may be denoted by $P(E)$ so that $dD(E) = P(E)\,dE$ and

$$P(E) = \frac{8\pi\bar{n}^3E^2[1 + (E/\bar{n})(d\bar{n}/dE)]}{h^3c^3[\exp(E/kT) - 1]}. \tag{3.2-16}$$

The spectral density has the units of the number of photons per unit volume and unit energy interval. The dispersion term $[1 + (E/\bar{n})(d\bar{n}/dE)]$ is often written as unity.

The Einstein Relations

Instead of two sharp levels for an atomic system, the available electron states in semiconductors are represented as a continuous band of states within the valence and conduction bands. In Fig. 3.2-2, an electron transition is represented. The transition is from a state E_1 within the valence band to a state E_2 within the conduction band and results from the absorption of a photon of energy $E_2 - E_1 = E_{21} = h\nu$. The rate for this process depends on several factors:

(1) the probability that the transition can occur, B_{12},
(2) the probability that the state E_1 contains an electron f_1,
(3) the probability that the state E_2 is empty $[1 - f_2]$, and
(4) the density of photons of energy E_{21}, $P(E_{21})$.

The upward transition rate may then be written as

$$r_{12} = B_{12}f_1[1 - f_2]P(E_{21}). \tag{3.2-17}$$

The occupation probability of E_1 is given by the Fermi–Dirac distribution for indistinguishable, identical particles with half-integral spin that obey

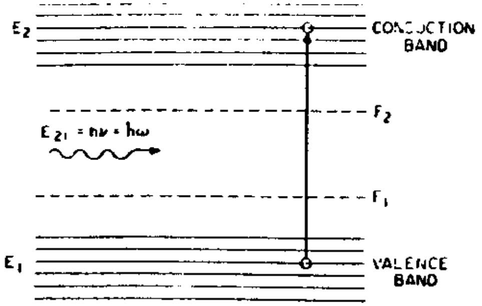


FIG. 3.2-2 Transition of an electron from E_1 to E_2 by the absorption of a photon of energy E_{21}. The quasi-Fermi levels for the valence and conduction bands are represented by F_1 and F_2, respectively.

the Pauli exclusion principle, and is[17]

$$f_1 = (\exp[(E_1 - F_1)/kT] + 1)^{-1}, \tag{3.2-18}$$

where F_1 represents the quasi-Fermi level for the valence band at nonequilibrium. Similarly, for the conduction band

$$f_2 = (\exp[(E_2 - F_2)/kT] + 1)^{-1}, \tag{3.2-19}$$

where F_2 is the quasi-Fermi level for the conduction band at nonequilibrium.

In addition to being absorbed, these photons can also stimulate the emission of a similar photon by the transition of an electron from E_2 to E_1. The downward transition rate for this process is

$$r_{21} = B_{21}f_2[1 - f_1]P(E_{21}), \tag{3.2-20}$$

where B_{21} is the transition probability, f_2 is the probability that E_2 is occupied and $[1 - f_1]$ represents the probability that E_1 is empty.

Also, electrons at E_2 can spontaneously return to E_1 without interaction with the radiation field $P(E_{21})$. The probability for this process is represented by A_{21}, and the spontaneous emission rate is given by

$$r_{21}(\text{spon}) = A_{21}f_2[1 - f_1]. \tag{3.2-21}$$

Several useful relationships can be established with Eqs. (3.2-17), (3.2-20), and (3.2-21).

At thermal equilibrium, the upward transition rate must equal the total downward transition rate

$$r_{12} = r_{21} + r_{21}(\text{spon}), \tag{3.2-22}$$

and $F_1 = F_2$. From Eqs. (3.2-17), (3.2-20), and (3.2-21), Eq. (3.2-22) becomes

$$P(E_{21}) = \frac{A_{21}f_2[1 - f_1]}{B_{12}f_1[1 - f_2] - B_{21}f_2[1 - f_1]}, \tag{3.2-23}$$

and by Eqs. (3.2-16), (3.2-18), and (3.2-19), this equation may be written as

$$\frac{8\pi\bar{n}^3E_{21}^2}{h^3c^3[\exp(E_{21}/kT) - 1]} = \frac{A_{21}}{B_{12}\exp(E_{21}/kT) - B_{21}}. \tag{3.2-24}$$

The $[1 + (h\nu/\bar{n})(d\bar{n}/dh\nu)]$ term in Eq. (3.2-24) has been written as unity. Also, it should be noted that the energy density distribution per unit frequency interval is often used instead of the photon density distribution per unit energy. For that case,[1,13,14] the left side of Eq. (3.2-24) is

$$\frac{8\pi\bar{n}^3h\nu^3}{c^3[\exp(h\nu/kT) - 1]}.$$

Equation (3.2-24) may be rewritten as

$$(8\pi\bar{n}^3E_{21}^2/h^3c^3)[B_{12}\exp(E_{21}/kT)-B_{21}]=A_{21}\exp(E_{21}/kT)-A_{21}, \quad (3.2\text{-}25)$$

and separated into temperature-dependent and temperature-independent terms. Equating the temperature independent terms gives

$$A_{21}=(8\pi\bar{n}^3E_{21}^2/h^3c^3)B_{21}. \quad (3.2\text{-}26)$$

and then equating the temperature dependent parts of Eq. (3.2-25) with A_{21} given by Eq. (3.2-26) gives

$$B_{12}=B_{21}. \quad (3.2\text{-}27)$$

Equations (3.2-26) and (3.2-27) are the Einstein relations and show that the spontaneous emission probability is related to the absorption and stimulated emission probability.

Necessary Condition for Stimulated Emission in Semiconductors

The necessary condition for stimulated emission was expressed very simply by Bernard and Duraffourg.[2] Stimulated emission in excess of absorption occurs when a photon is more likely to cause a downward transition of an electron from the conduction band with the emission of a photon than the upward transition from the valence to conduction band with absorption of the photon. This condition requires that r_{21}, as given by Eq. (3.2-20), must exceed r_{12}, as given by Eq. (3.2-17), so that

$$B_{21}f_2[1-f_1]P(E_{21})>B_{12}f_1[1-f_2]P(E_{21}). \quad (3.2\text{-}28)$$

Since Eq. (3.2-27) gave $B_{12}=B_{21}$, this condition is

$$f_2[1-f_1]>f_1[1-f_2]. \quad (3.2\text{-}29)$$

with f_1 and f_2 given by Eqs. (3.2-18) and (3.2-19). Equation (3.2-29) then reduces to

$$\exp[(F_2-F_1)/kT]>\exp[(E_2-E_1)/kT]. \quad (3.2\text{-}30)$$

or more simply.

$$F_2-F_1>E_2-E_1. \quad (3.2\text{-}31)$$

Therefore, the separation of the quasi-Fermi levels must exceed the photon emission energy for the downward stimulated emission rate to exceed the upward absorption rate.

The Net Stimulated Emission Rate

A frequently used quantity is the net stimulated emission rate $r_{21}(\mathrm{stim})$, which is the difference between the downward transition rate r_{21} and the upward transition rate r_{12}. From Eqs. (3.2-17) and (3.2-20) this difference is

$$r_{21}(\mathrm{stim})=B_{21}f_2[1-f_1]P(E_{21})-B_{12}f_1[1-f_2]P(E_{21}), \quad (3.2\text{-}32)$$

and since $B_{12}=B_{21}$, this expression becomes

$$r_{21}(\mathrm{stim})=B_{12}P(E_{21})[f_2-f_1]. \quad (3.2\text{-}33)$$

From Eqs. (3.2-16) and (3.2-26), this relation reduces to

$$r_{21}(\mathrm{stim})=\frac{A_{21}[f_2-f_1]}{\exp(E_{21}/kT)-1} \quad (3.2\text{-}34)$$

In Eq. (3.2-34) it has become common usage[18] to define $A_{21}[f_2-f_1]$ as the stimulated emission rate $r_{\mathrm{stim}}(E_{21})$ because of its similarity in form to the spontaneous rate in Eq. (3.2-21):

$$r_{\mathrm{stim}}(E_{21})=A_{21}[f_2-f_1]. \quad (3.2\text{-}35)$$

The units of r_{stim} are the number of photons per unit volume per second per energy interval.

It is important to note that three rather similar designations are used for the stimulated emission rate. There are

(1) r_{21}, the downward transition rate for stimulation of a similar photon,

(2) $r_{21}(\mathrm{stim})$, the net stimulated emission rate, which is the difference between the downward transition rate r_{21} and the upward transition rate r_{12}, and

(3) $r_{\mathrm{stim}}(E_{21})$, the quantity generally called the stimulated emission rate and when $r_{\mathrm{stim}}(E_{21})$ is multiplied by the number of photons per state $[\exp(E_{21}/kT)-1]^{-1}$, it becomes the net stimulated emission rate $r_{21}(\mathrm{stim})$.

The Absorption Coefficient

The interaction of photons and electrons in the solid may be related to a macroscopic property, the absorption coefficient α. The net absorption rate is the difference between the upward transition rate r_{12} and the downward transition rate r_{21}. From Eqs. (3.2-17) and (3.2-20) this difference is

$$r_{12}(\mathrm{abs})=B_{12}f_1[1-f_2]P(E_{21})-B_{21}f_2[1-f_1]P(E_{21}), \quad (3.2\text{-}36)$$

and again with $B_{12}=B_{21}$ this expression becomes

$$r_{12}(\mathrm{abs})=B_{12}[f_1-f_2]P(E_{21}), \quad (3.2\text{-}37)$$

where $B_{12}[f_1-f_2]$ is the net absorption probability.

The net absorption rate $r_{12}(\mathrm{abs})$ is the absorption coefficient times the photon flux $F(E)$. The photon flux is simply the photon density distribution $P(E)$ given by Eq. (3.2-16) times the group velocity v_g. The group velocity in the dielectric medium is [see Eq. (3.2-11) for dk and Eq. (3.2-4) for $\omega = 2\pi E/h$]

$$v_g = \frac{d\omega}{dk} = \frac{2\pi\, dE}{h\, dk} = \frac{c/\bar{n}}{1 + (E/\bar{n})(d\bar{n}/dE)}. \tag{3.2-38}$$

Therefore, the absorption coefficient may be written as

$$\alpha(E_{21}) = \frac{r_{12}(\text{abs})}{F(E_{21})} = \frac{r_{12}(\text{abs})}{P(E_{21})v_g} = \frac{B_{12}[f_1 - f_2]}{c/\bar{n}}, \tag{3.2-39}$$

where the $[1 + (E/\bar{n})(d\bar{n}/dE)]$ dispersion term in v_g has been taken as unity.

The absorption coefficient may be related to the stimulated emission $r_{\text{stim}}(E_{21})$. Equation (3.2-26) permits writing Eq. (3.2-35) as

$$-r_{\text{stim}}(E_{21}) = (8\pi\bar{n}^3E_{21}^3/h^3c^3)B_{12}[f_1 - f_2], \tag{3.2-40}$$

so that $\alpha(E)$ becomes

$$\alpha(E_{21}) = -(h^3c^2/8\pi\bar{n}^2E_{21}^2)r_{\text{stim}}(E_{21}). \tag{3.2-41}$$

The units for $\alpha(E_{21})$ are cm^{-1}. Equation (3.2-41) shows that $\alpha(E_{21})$ and $r_{\text{stim}}(E_{21})$ are related by the constant prefactor.

Relation of Spontaneous Emission to the Absorption Coefficient

Because of the Einstein relation given by Eq. (3.2-26), the spontaneous emission rate may be written in terms of the absorption coefficient. With Eq. (3.2-37) for $r_{12}(\text{abs})$ in Eq. (3.2-39),

$$B_{12}[f_1 - f_2]P(E_{21}) = \alpha(E_{12})P(E_{21})v_g, \tag{3.2-42}$$

and by Eqs. (3.2-21) and (3.2-26),

$$r_{21}(\text{spon}) = (8\pi\bar{n}^3E_{21}^3/h^3c^3)B_{21}f_2[1 - f_1] = r_{\text{spon}}(E_{21}). \tag{3.2-43}$$

Equation (3.2-42) permits elimination of B_{21} in Eq. (3.2-43). With $v_g = c/\bar{n}$, $r_{\text{spon}}(E_{21})$ becomes

$$r_{\text{spon}}(E_{21}) = \frac{8\pi\bar{n}^2E_{21}^2}{h^3c^2}\,\alpha(E_{21})\,\frac{f_2[1 - f_1]}{[f_1 - f_2]}, \tag{3.2-44}$$

or

$$r_{\text{spon}}(E_{21}) = \frac{8\pi\bar{n}^2E_{21}^2\alpha(E_{21})}{h^3c^2\{\exp[E_{21} - (F_2 - F_1)]/kT - 1\}}. \tag{3.2-45}$$

The units for $r_{\text{spon}}(E_{21})$ are number of photons per unit volume per second per energy interval, and the identity of Eq. (3.2-43) was made to maintain notational uniformity.

Relation Between the Spontaneous and Stimulated Emission Rates

Equations (3.2-41) and (3.2-45) relate $r_{\text{stim}}(E_{21})$ and $r_{\text{spon}}(E_{21})$ to $\alpha(E_{21})$. Therefore, the stimulated emission rate, as defined by Eq. (3.2-35), may readily be related to the spontaneous emission rate

$$r_{\text{spon}}(E_{21}) = -\frac{r_{\text{stim}}(E_{21})}{\{\exp[E_{21} - (F_2 - F_1)]/kT - 1\}}, \tag{3.2-46}$$

or

$$r_{\text{stim}}(E_{21}) = r_{\text{spon}}(E_{21})\{1 - \exp[E_{21} - (F_2 - F_1)]/kT\}. \tag{3.2-47}$$

These expressions in Eqs. (3.2-41), (3.2-45), and (3.2-47) demonstrate that $\alpha(E)$, $r_{\text{spon}}(E)$, and $r_{\text{stim}}(E)$ are related to each other and that knowledge of one gives the other two. To evaluate these expressions, one quantity such as $\alpha(E)$ must be obtained experimentally or the transistion probabilities B_{12} or A_{21} must be calculated. Therefore, in the next section of this chapter expressions are considered for $\alpha(E)$, $r_{\text{spon}}(E)$, and $r_{\text{stim}}(E)$ that have the transition probabilities and the distribution of states representative of semiconductors.

3.3 TRANSITION PROBABILITY

Fermi's "Golden Rule"

Since Eq. (3.2-45) shows that $r_{\text{spon}}(E)$ can be found from $\alpha(E)$ and that Eq. (3.2-47) relates $r_{\text{spon}}(E)$ to $r_{\text{stim}}(E)$, it is only necessary to determine $\alpha(E)$ to obtain the spontaneous and stimulated emission rates. Also, calculated values of $\alpha(E)$ may readily be verified by experimental measurements. For these reasons, only $\alpha(E)$ will be considered in the analysis that follows. For photon absorption between two discrete levels, the absorption coefficient was given as

$$\alpha(E_{21}) = B_{12}[f_1 - f_2]\bar{n}/c. \tag{3.2-39}$$

In this expression the transition probability B_{12} is unknown, and it can be expected to depend on various properties of the system that relate the interaction of electrons in the solid with electromagnetic radiation. This interaction requires recourse to quantum mechanics in order to evaluate B_{12}.

Consideration of the interaction between electrons in the semiconductor and electromagnetic radiation requires the techniques of time-dependent perturbation theory.[3] With this procedure, the properties of the system are determined in the absence of radiation, and the alteration that occurs with the radiation is then calculated. If convergent techniques can be used for the perturbation effects, solutions can then be obtained for the actual problem. Rather than go through the straightforward but lengthly analysis, the well-known result referred to as Fermi's "Golden Rule" will be given. Solution of the Schrödinger equation with a perturbation harmonic in time of the form

$$H^1(\mathbf{r},t) = H^1(\mathbf{r})\cos\omega t \tag{3.3-1}$$

gives the transition probability as[3]

$$B_{12} = (\pi/2h)|\langle\Psi_1^*(\mathbf{r},t)|H^1|\Psi_2(\mathbf{r},t)\rangle|^2, \tag{3.3-2}$$

which is called Fermi's Golden Rule. In Eq. (3.3-2), **r** is the three-dimensional spatial vector, $\Psi_1^*(\mathbf{r},t)$ the complex conjugate of the wave function of the initial state, H^1 the interaction Hamiltonian, and $\Psi_2(\mathbf{r},t)$ the wave function of the final state. The transition probability from Fermi's Golden Rule has also been given by Stern[19] and by Bebb and Williams.[20]

The quantity $\langle\Psi_1^*(\mathbf{r},t)|H^1|\Psi_2(\mathbf{r},t)\rangle$ is commonly called the matrix element of the interaction Hamiltonian H^1 between $\Psi_1^*(\mathbf{r},t)$ and $\Psi_2(\mathbf{r},t)$. As will be shown later, H^1 is essentially ∇, the familiar differential operator. Therefore, the matrix element is the scalar product of the initial state wave function $\Psi_1^*(\mathbf{r},t)$ with the function that results from the operation of H^1 (differentiation) on the final-state wave function $\Psi_2(\mathbf{r},t)$. The matrix element is given by[3]

$$\langle\Psi_1^*(\mathbf{r},t)|H^1|\Psi_2(\mathbf{r},t)\rangle = \int_V \Psi_1^*(\mathbf{r},t)H^1\Psi_2(\mathbf{r},t)\,d^3\mathbf{r}. \tag{3.3-3}$$

The remainder of this section is devoted to the determination and evaluation of the interaction Hamiltonian in the matrix element.

The Interaction Hamiltonian

In this part of Section 3.3, the quantities that enter the interaction Hamiltonian in Eq. (3.3-3) are illustrated and described. The text by White[3] discusses very thoroughly the concepts to be briefly presented here and should be consulted for further description.

In quantum mechanics, the description of the particle is contained in its wave function $\Psi(\mathbf{r},t)$. This state function contains all the information about the system. The behavior of $\Psi(\mathbf{r},t)$ as a function of spatial coordinates and time is given by the Schrödinger wave equation

$$H_{op}\Psi(\mathbf{r},t) = -(h/j)[\partial\Psi(\mathbf{r},t)/\partial t], \tag{3.3-4}$$

where H_{op}, as described in the following, is the operator associated with the system Hamiltonian.

The system Hamiltonian refers to the total energy of the system. The classical Hamiltonian for a particle is a conservative force and is the sum of the kinetic and potential energy

$$H = (p^2/2m) + V(\mathbf{r}), \tag{3.3-5}$$

where m is the particle mass. A conservative force is one that is derivable from a single-valued potential, that is, $\mathbf{F} = -\nabla V(\mathbf{r})$. It requires the potential of a particle at a given point to be independent of the path by which the particle reached that point. This requirement implies that the potential of the particle is independent of its velocity at that point. For force due to the electromagnetic field, it will be necessary to consider a nonconservative force on an electron.

A mathematical operator such as H_{op} may be associated with physically observable quantities such as $\Psi(\mathbf{r},t)$. From the properties of the operator, it is possible to obtain the behavior of $\Psi(\mathbf{r},t)$. For example, in the one-dimension x, the expression $\partial\Psi(x,t)/\partial x$ can be considered as composed of the operator $\partial/\partial x$ and the operand $\Psi(x,t)$. The operator associated with the momentum **p** becomes[3]

$$\mathbf{p} \rightarrow (h/j)\nabla \tag{3.3-6}$$

so that the classical Hamiltonian operator H_{op}^{c} becomes

$$H_{op}^{c} = -(h^2\nabla^2/2m) + V(\mathbf{r}). \tag{3.3-7}$$

With Eq. (3.3-7), Eq. (3.3-4) becomes

$$[-(h^2/2m)\nabla^2 + V(\mathbf{r})]\Psi(\mathbf{r},t) = -(h/j)[\partial\Psi(\mathbf{r},t)/\partial t]. \tag{3.3-8}$$

This equation may be separated into two equations, one involving spatial variables and one involving time. The separation of variables was illustrated in Section 2.4 for the wave equation. As for the waveguide problem, application of boundary conditions will lead to eigenvalue equations, and the system eigenvalues are products of a spatial eigenfunction and a harmonic time function

$$\Psi_n(\mathbf{r},t) = \psi_n(\mathbf{r})\exp(j\omega_n t). \tag{3.3-9}$$

Next, consider the Hamiltonian for the interaction of electromagnetic radiation with an electron (see Chapter 2 of Ref. 3). The force on the electron of charge q moving with the velocity **v** in an electromagnetic field is given by the Lorentz force

$$\mathbf{F} = q(\mathscr{E} + \mathbf{v} \times \mathscr{B}). \tag{3.3-10}$$

Since **F** depends on **v**, this case is nonconservative, and **F** cannot be obtained from the gradient of a scalar field. For the nonconservative force, it is convenient to represent the electromagnetic field by the vector field **A**.

This field is found from Maxwell's equations that were given in Section 2.2:

$$\nabla \times \mathscr{E} = -\partial \mathscr{B}/\partial t \tag{2.2-1}$$

and

$$\nabla \cdot \mathscr{B} = 0. \tag{2.2-7}$$

From vector algebra, the divergence of the curl of a vector is zero, i.e.,

$$\nabla \cdot \nabla \times \mathbf{G} = 0, \tag{3.3-11}$$

and by Eq. (2.2-7), $\nabla \cdot \mathscr{B} = 0$. Therefore, $\mathscr{B}$ is the curl of some vector defined as $\mathbf{A}$:

$$\mathscr{B} = \nabla \times \mathbf{A}. \tag{3.3-12}$$

Equation (2.2-1) becomes

$$\nabla \times \mathscr{E} = -(\partial/\partial t)\nabla \times \mathbf{A} \tag{3.3-13}$$

and

$$\nabla \times (\mathscr{E} + (\partial/\partial t)\mathbf{A}) = 0. \tag{3.3-14}$$

Also, from vector algebra, if the curl of some vector is zero, then this vector must be the gradient of a potential φ, and

$$\mathscr{E} + (\partial/\partial t)\mathbf{A} = -\nabla\varphi. \tag{3.3-15}$$

The vector $\mathbf{A}$ and scalar φ may be chosen so that $\varphi = 0$ and

$$\mathscr{E} = -\partial \mathbf{A}/\partial t. \tag{3.3-16}$$

Although not derived here, the Hamiltonian for the electron moving in the nonconservative potential is given by the well-known expression (see Chapter 2 of Ref. 3)

$$H = (1/2m)(\mathbf{p} - q\mathbf{A})^2 + V(\mathbf{r}), \tag{3.3-17}$$

where Eq. (3.3-12) defined $\mathbf{A}$, and Eq. (3.3-16) related $\mathbf{A}$ to $\mathscr{E}$.

The interaction Hamiltonian is then obtained by writing out the squared term in Eq. (3.3-17) as

$$H = (1/2m)(\mathbf{p}^2 - 2q\mathbf{A} \cdot \mathbf{p} + q^2\mathbf{A}^2) + V(\mathbf{r}). \tag{3.3-18}$$

The higher-order term $q^2\mathbf{A}^2$ is neglected, and by Eq. (3.3-6) the operator H_{op} becomes

$$H_{op} = (1/2m)(-\hbar^2\nabla^2 - 2(q\hbar/j)\mathbf{A} \cdot \nabla) + V(\mathbf{r}). \tag{3.3-19}$$

Comparing this operator with H_{op} for the classical Hamiltonian in Eq. (3.3-7) gives

$$H_{op} = H^0_{op} + H^1_{op}, \tag{3.3-20}$$

where

$$H^1_{op} = -(q\hbar/jm)\mathbf{A} \cdot \nabla, \tag{3.3-21}$$

or

$$H^1 = -(q/m)\mathbf{A} \cdot \mathbf{p}. \tag{3.3-22}$$

Equation (3.2-22) defines the interaction Hamiltonian given in operator form in Eq. (3.3-21).

The Matrix Element

The expression for the matrix element in Eq. (3.3-3) with H^1 given by Eq. (3.3-22) can be further simplified by representation of the vector potential by the electric field. The electric field for a traveling wave may be written as [see Eq. (2.2-27)]

$$\mathscr{E} = \mathbf{a}_x\mathscr{E}_0\cos(\omega t - kz) = \mathbf{a}_x\mathscr{E}_0\exp[j(\omega t - kz)], \tag{3.3-23}$$

where the $\mathrm{Re}\{\exp[j(\omega t - kz)]\}$ is implied for $\exp[j(\omega t - kz)]$ as described in Section 2.2. In Eq. (3.3-23), the electric field is polarized parallel to the x-axis with wave vector k. For the cubic crystals to be considered here, the direction of polarization is unimportant. The vector field $\mathbf{A}$ is related to $\mathscr{E}$ by Eq. (3.3-16) so that

$$\mathbf{A} = (j\mathbf{a}_x\mathscr{E}_0/\omega)\exp[j(\omega t - kz)], \tag{3.3-24}$$

and

$$|\mathbf{A}|^2 = |\mathbf{A} \cdot \mathbf{A}^*|^2 = \mathscr{E}_0{}^2/\omega^2. \tag{3.3-25}$$

To evaluate the magnitude of the electric field $\mathscr{E}_0$, the electromagnetic flux as given by the real part of the Poynting vector may be related to the photon energy $E = \hbar\omega$. From Eq. (2.2-57) the Poynting vector $|\mathbf{S}|$ in exponential notation is

$$|\mathbf{S}| = \tfrac{1}{2}\,\mathrm{Re}(\mathscr{E} \times \mathscr{H}^*), \tag{2.2-57}$$

and for $\mathscr{E}$ given by Eq. (3.3-23), $\mathscr{H}$ is given by Eq. (2.2-14) as

$$\mathscr{H}_y = (\mathbf{a}_y\mathscr{E}_0 k/\mu_0\omega)\exp[j(\omega t - kz)], \tag{3.3-26}$$

and

$$|\mathbf{S}| = \tfrac{1}{2}(\mathscr{E}_0{}^2 k/\mu_0\omega). \tag{3.3-27}$$

The flux magnitude for a photon is also given by the photon energy $\hbar\omega$ times the group velocity $c/\bar{n}$ so that

$$\hbar\omega c/\bar{n} = \tfrac{1}{2}\bar{n}\varepsilon_0\mathcal{E}_0^{\,2}c. \qquad (3.3\text{-}28)$$

where Eq. (3.3-27) has been rewritten with $k = \bar{n}\omega/c$ and $c^2 = 1/\mu_0\varepsilon_0$. By Eqs. (3.3-25) and (3.3-28),

$$|\mathbf{A}|^2 = 2\hbar/\varepsilon_0\bar{n}^2\omega. \qquad (3.3\text{-}29)$$

For the more general three-dimensional polarization vector $\mathbf{n}$, the same $|\mathbf{A}|^2$ results as Eq. (3.3-29), but $\mathbf{A}$ of Eq. (3.3-24) becomes

$$\mathbf{A} = (\mathbf{n}\mathcal{E}_0/\omega)\exp[j(\omega t - \mathbf{k}\cdot\mathbf{r})]. \qquad (3.3\text{-}30)$$

The transition probability given by Eq. (3.3-2) may now be written with Eq. (3.3-9) for the wave functions, Eq. (3.3-22) for the interaction Hamiltonian, and Eq. (3.3-30) for the vector potential as

$$B_{12} = \frac{\pi}{2\hbar}\left|\left\langle \psi_1^*(\mathbf{r})\exp(-j\omega_1 t)\right| - \mathbf{n}\frac{q}{m}\left(\frac{2\hbar}{\varepsilon_0\bar{n}^2\omega}\right)^{1/2}\right.$$
$$\left.\times \exp[j(\omega t - \mathbf{k}\cdot\mathbf{r})]\cdot\mathbf{p}\left|\psi_2(\mathbf{r})\exp(j\omega_2 t)\right\rangle\right|^2. \qquad (3.3\text{-}31)$$

For the harmonic condition that $\omega = \omega_2 - \omega_1$, the exponential time dependences goes to unity, and this expression may be written as

$$B_{12} = \frac{\pi q^2\hbar}{m^2\varepsilon_0\bar{n}^2\hbar\omega}|\langle\psi_1^*(\mathbf{r})\,\mathbf{p}\,\psi_2(\mathbf{r})\rangle|^2, \qquad (3.3\text{-}32)$$

where $\exp(-j\mathbf{k}\cdot\mathbf{r})$ has been taken as unity because the range of $\mathbf{r}$ where $\psi_1^*(\mathbf{r})$ and $\psi_2(\mathbf{r})$ have value is very small compared to λ, i.e., $\mathbf{k}\cdot\mathbf{r} \ll 1$. The momentum $\mathbf{p}$ is utilized in its operator form of Eq. (3.3-6). The expression in brackets is called the momentum matrix element M, and in the same manner as for Eq. (3.3-3)

$$M = \langle\Psi_1^*(\mathbf{r})|\mathbf{p}|\Psi_2(\mathbf{r})\rangle = \int_V \Psi_1^*(\mathbf{r})\mathbf{p}\Psi_2(\mathbf{r})d^3\mathbf{r}. \qquad (3.3\text{-}33)$$

The transition probability now becomes

$$B_{12} = \frac{\pi q^2\hbar}{m^2\varepsilon_0\bar{n}^2\hbar\omega}|M|^2. \qquad (3.3\text{-}34)$$

The expressions in Eq. (3.3-33) are often called the dipole matrix element because they correspond to a term of the form $\mathcal{E}\cdot\mathbf{d}$ where $\mathbf{d}$ is the dipole moment. Although it is not at all obvious, it can be shown[3] that Eq. (3.3-33) gives the electric-dipole interaction, and hence it has become named the dipole matrix element as well as the momentum matrix element. Also, the quantity $2|M|^2/\hbar\omega m$ is called the oscillator strength.[19]

3.4 OPTICAL ABSORPTION AND EMISSION RATES IN SEMICONDUCTORS

Density of States

The absorption and emission rates considered in Sections 3.2 and 3.3 represent transitions for the entire system between pairs of discrete energy levels separated by $\hbar\omega_{21}$. Extension of these expressions must now be made to include the various states within the valence and conduction bands of the semiconductor. The single-electron approximation is made, and the transition is considered as the change in state of a single electron. Elementary discussions of the single-electron approximation have been given in numerous texts, such as the books by Blakemore,[21] McKelvey,[22] and Bube,[23] and will not be repeated here.

The density of single-electron states per unit energy for the conduction band is given by the familiar parabolic expression[22]

$$\rho_c(E - E_c) = (2\pi^2)^{-1}(2m_n/\hbar^2)^{3/2}(E - E_c)^{1/2}, \qquad (3.4\text{-}1)$$

where m_n is the effective mass for electrons in the conduction band and E_c is the conduction band edge. Similarly, for the valence band[22]

$$\rho_v(E_v - E) = (2\pi^2)^{-1}(2m_p/\hbar^2)^{3/2}(E_v - E)^{1/2}, \qquad (3.4\text{-}2)$$

where m_p is the effective mass for holes in the valence band, and E_v is the valence band edge. An example of the density of states for a conduction band with an effective electron mass $m_n = 0.07m_0$, where m_0 is the free electron mass, and for a valence band with an effective hole mass $m_p = 0.5m_0$ is shown in Fig. 3.4-1a. The energy gap E_g is the separation $(E_c - E_v)$ between the valence and conduction bands. These effective masses represent GaAs, which will be considered in detail later in this chapter. The energy gap has been taken as 0.5 eV for convenience in plotting.

The Absorption Coefficient

In Eq. (3.2-17), the upward transition rate between states 1 and 2 was taken to be proportional to the probability f_1 that the state E_1 contains an electron. For transitions between the valence and conduction bands of a semiconductor, the rate depends on the density of filled states in the valence band $\rho_1(E)f_1$. Similarly, the empty-state probability in the conduction band $[1 - f_2]$ becomes the density of empty states $\rho_2(E)[1 - f_2]$. The occupation

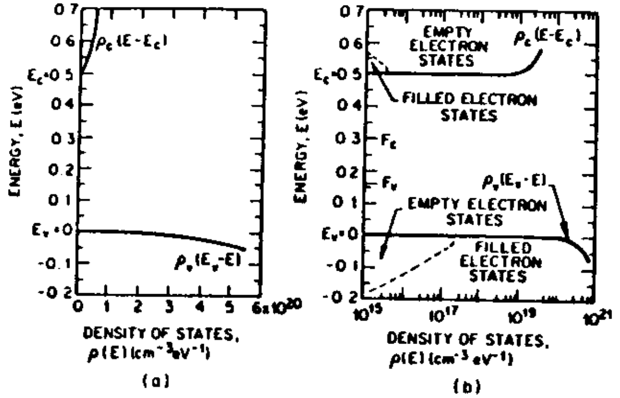


FIG. 3.4-1 (a) The variation of the parabolic density of states with energy for $m_e = 0.07m_0$ and $m_p = 0.5m_0$. (b) The distribution of holes in the valence band and electrons in the conduction band for $p = 1 \times 10^{16}$ cm^{-3} and $n = 1 \times 10^{14}$ cm^{-3} at $T = 297$°K.

probabilities were given in Eqs. (3.2-18) and (3.2-19). These densities of filled and empty states become

$$\rho_1(E)f_1 = \rho_v(E_v - E)f_v, \qquad (3.4\text{-}3)$$

and

$$\rho_2(E)[1 - f_2] = \rho_c(E - E_c)[1 - f_c]. \qquad (3.4\text{-}4)$$

The densities of filled and empty states are illustrated in Fig. 3.4-1b for the effective mass values used in Fig. 3.4-1a. For the valence band, $p = 1 \times 10^{16}$ cm^{-3}, and for the conduction band, $n = 1 \times 10^{14}$ cm^{-3}. To obtain these curves in Fig. 3.4-1b, $\rho_v(E_v - E)$ of Fig. 3.4-1a is multiplied by f_v of Eq. (3.2-18), and $\rho_c(E - E_c)$ of Fig. 3.4-1a is multiplied by f_c of Eq. (3.2-19). The quasi-Fermi levels F_v and F_c are obtained in the manner described in Section 4.3. To illustrate both the density of filled and empty states, it is necessary to use the semilogarithmic plot.

The absorption coefficient is proportional to the difference between the upward transition rate and the downward transition rate and was given by Eq. (3.2-39) for two discrete levels. In a semiconductor, instead of two discrete levels there is a continuum of states in the conduction and valence bands characterized by the density of states $\rho_c(E - E_c)$ and $\rho_v(E_v - E)$ that are given in Eqs. (3.4-1) and (3.4-2). Therefore, the absorption coefficient must be the sum of the absorption coefficients at $\hbar\omega$ for all of the energy levels separated by $\hbar\omega$. The sum becomes the integral

$$\alpha(\hbar\omega) = \int_{-\infty}^{\infty} \frac{B_{12}}{c/\bar{n}}[f_1 - f_2]\rho_v(E_v - E)\rho_c(E - E_c)\delta(E_2 - E_1 - \hbar\omega)\,dE. \qquad (3.4\text{-}5)$$

In Eq. (3.4-5), the integral is taken over the products of $\rho_v(E_c - E_1)$ and $\rho_c(E_2 - E_c)$ of the various E_2 and E_1 in the conduction and valence bands that are separated by a given photon energy $\hbar\omega$. Note that the delta function $\delta(E_2 - E_1 - \hbar\omega)$ is used to specify that $\rho_v(E_v - E_1)$ and $\rho_c(E_2 - E_c)$ are separated by $\hbar\omega$.

Because most of the literature on this subject is by Stern, his notation will be used. When writing the integral in Eq. (3.4-5), it is convenient to shift the valence band upward by $\hbar\omega$, as illustrated in the next part of this section for the spontaneous emission rate. In this case, the photon energy $\hbar\omega$ is designated by E, and E' becomes the energy variable with $E' = 0$ at E_c, and $E'' = E' - \hbar\omega$. Therefore $\rho_c(E - E_c)$ becomes $\rho_c(E')$ and $\rho_v(E_v - E)$ is shifted upward by $\hbar\omega$ and becomes $\rho_v(E'')$. With Eq. (3.3-34) for B_{21}, the expression for the absorption coefficient in Eq. (3.4-5) becomes[8]

$$\alpha(E) = (\pi q^2 h/\varepsilon_0 m^2 c\bar{n}E)\int_{-\infty}^{\infty} \rho_c(E')\rho_v(E'')|M(E', E'')|^2[f(E'') - f(E')]\,dE',$$
$$(3.4\text{-}6)$$

where ε_0 is replaced by $\varepsilon_0/4\pi$ for cgs units. When several valence bands are present, as for III–V semiconductors, both the heavy-hole and light-hole band must be included. The absorption coefficient is then given by the sum of terms like Eq. (3.4-6) for each valence band.

The Spontaneous Emission Rate

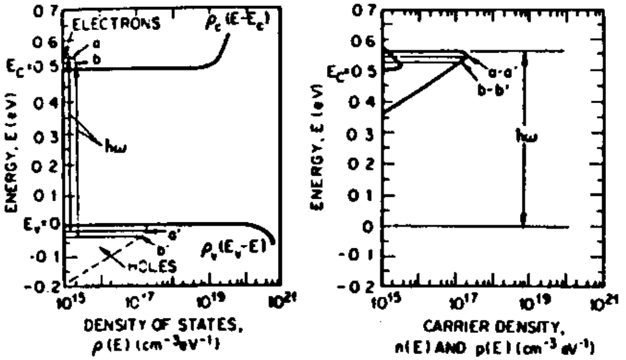
The probability of spontaneous emission A_{21} was related to B_{12} through the Einstein relations given by Eqs. (3.2-26) and (3.2-27). With B_{12} given by Eq. (3.3-34), A_{21} becomes

$$A_{21} = \frac{4\pi\bar{n}q^2 E_{21}}{m^2\varepsilon_0 h^2 c^3}|M|^2. \qquad (3.4\text{-}7)$$

The spontaneous emission rate between two discrete levels E_2 and E_1 was given by Eq. (3.2-21). In the same manner as for the absorption coefficient, the spontaneous emission rate depends on the density of filled conduction band states and the density of empty valence band states and may be written as[8]

$$r_{\text{spon}}(E) = \frac{4\pi\bar{n}q^2 E}{m^2\varepsilon_0 h^2 c^3}\int_{-\infty}^{\infty} \rho_c(E')\rho_v(E'')|M(E', E'')|^2 f(E')[1 - f(E'')]\,dE',$$
$$(3.4\text{-}8)$$

where the photon emission energy $E = E' - E''$ as for Eq. (3.4-6). The density of empty valence band states (holes) $p(E) = \rho_v(E_v - E)[1 - f_v]$ and filled conduction band states (electrons) $n(E) = \rho_c(E - E_c)f_c$ that are separated by $\hbar\omega$ are illustrated in Fig. 3.4-2a. In the evaluation of Eq. (3.4-8), the hole



(a) (b)

FIG. 3.4-2 (a) Representation of the empty valence band states (holes) and filled conduction band states (electrons) at 297°K. The integral in Eq. (3.4-8) sums the emission between pairs of states a–a′ and b–b′ separated by $\hbar\omega$. (b) Representation of the evaluation of the spontaneous emission rate by Eq. (3.4-8). The hole distribution has been shifted upward by $\hbar\omega$, and the integral contains the product of the overlapping of these electron and hole distributions.

distribution is shifted upward by $\hbar\omega$ as illustrated in Fig. 3.4-2b. The location of $p(E)$ with respect to $n(E)$ will differ for each value of photon energy $\hbar\omega$.

The Stimulated Emission Rate

The stimulated emission rate between two discrete levels E_2 and E_1 was given by Eq. (3.2-35) and contains the same probability A_{21} as spontaneous emission. With Eq. (3.4-7) for A_{21}, the stimulated emission rate depends on the difference between the density of filled conduction and valence band states and may be written as

$$r_{\text{stim}}(E) = \frac{4\pi\bar{n}q^2E}{m^2\varepsilon_0 h^2c^3}\int_{-\infty}^{\infty}\rho_c(E')\rho_v(E'')|M(E',E'')|^2[f(E')-f(E'')]\,dE'. \quad (3.4\text{-}9)$$

Except for the Fermi factors, Eq. (3.4-8) for the spontaneous emission rate and Eq. (3.4-9) for the stimulated emission rate are identical. The net stimulated emission rate $r_\ell(\text{stim})$ [see Eq. (3.2-34)] is Eq. (3.4-9) multiplied by the number of photons per state $[\exp(E/kT)-1]^{-1}$. It should be emphasized that quasi-equilibrium is assumed to exist within the conduction and valence bands for Eqs. (3.4-6), (3.4-8), and (3.4-9). In several papers, departure from quasi-equilibrium has been suggested to explain certain unexpected features of their results.[24–27] However, at room temperature the equivalence between steady-state and time-resolved spectra demonstrated that quasi-equilibrium exists within the conduction and valence bands.[28]

The problem of evaluating $\alpha(E)$, $r_{\text{spon}}(E)$, or $r_{\text{stim}}(E)$ becomes one of evaluating $\rho_c(E')$, $\rho_v(E'')$, and $|M(E',E'')|^2$. At the high impurity concentrations or excitation levels encountered for semiconductor lasers, the density of states are concentration dependent and cannot be represented by the simple parabolic expression of Eqs. (3.4-1) and (3.4-2). The concentration dependence of the density of states is considered in Section 3.5. The evaluation of the matrix element is then discussed in Section 3.6.