

Appendix A: k.p Method

A.1 Band Theory: Bloch Functions

A solid consists of many atoms and electrons. The total energy of the system is therefore the sum of the kinetic energies of all the nuclei and electrons, the potential energy due to nuclear forces, the potential energies of electrons in the field of nuclei, the potential energy due to electron–electron interactions, and the magnetic energy associated with the spin and the orbit. The total Hamiltonian of the system may be constructed accordingly. The formidable problem of solving the resultant Schrödinger equation is bypassed by introducing several approximations. Since the motion of nuclei is sluggish, the electrons instantaneously adjust their motion to that of the ions. The total wavefunction is then written as a wavefunction for ions $\phi(\mathbf{R})$ and that for all electrons $\psi(r, \mathbf{R})$ instantaneously dependent on all ionic positions \mathbf{R} . An approximation, known as the *adiabatic approximation*, is introduced to decouple the Schrödinger equation into a purely ionic and a purely electronic equation, which are expressed, respectively, as

$$H_L \phi(\mathbf{R}) = E_L \phi(\mathbf{R}) \quad (\text{A.1})$$

and

$$H_e \psi(\mathbf{r}, \mathbf{R}) = E_e \psi(r, \mathbf{R}) \quad (\text{A.2})$$

where \mathbf{r} denotes the electronic coordinates [1, 2].

The electron potential energy is due to electron–electron and electron–ion interactions. If a suitable average is found for the first, a constant repulsive contribution can be added to the electron energy and then each electron becomes independent. The one-electron Schrödinger equation then takes the form

$$H_{ei} \psi_i(\mathbf{r}_i, \mathbf{R}) = E_{ei} \psi_i(\mathbf{r}_i, \mathbf{R}) \quad (\text{A.3})$$

where

$$H_{ei} = \frac{\mathbf{p}_i^2}{2m_0} + \sum_i V(\mathbf{r}_i, \mathbf{R}_i) \quad (\text{A.4})$$

and \mathbf{p}_i is the momentum of the i th electron. The Hamiltonian still depends on the fluctuating position of the ion. In the next approximation, the ions are assumed to lie in their equilibrium position and the effect of ionic vibration is taken as a perturbation. Thus the problem is reduced to solving the equation

$$\frac{\mathbf{p}^2}{2m_0} + \sum_i V(\mathbf{r} - \mathbf{R}_{i0})\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad (\text{A.5})$$

The ionic potential V is periodic and the eigenfunctions are Bloch functions expressed as

$$\psi_{n\mathbf{k}}(\mathbf{r}) = U_{n\mathbf{k}}(r) \exp(j\mathbf{k} \cdot \mathbf{r}), \quad (\text{A.6})$$

where the cell periodic part $U(\mathbf{r})$ obeys the relation

$$U_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = U_{n\mathbf{k}}(\mathbf{r}). \quad (\text{A.7})$$

In the above equations, \mathbf{R} is a vector of the Bravais lattice, n denotes the band index, and \mathbf{k} is a wave vector of the electron in the first Brillouin zone. From Eqs. (A.6) and (A.7)

$$\psi_{n\mathbf{k}}(\mathbf{r} + \mathbf{R}) = \psi_{n\mathbf{k}}(\mathbf{r}) \exp(j\mathbf{k} \cdot \mathbf{R})$$

The Bloch functions are eigenfunctions of the one-electron Schrödinger equation and therefore they are orthogonal to one another. Thus

$$\int \psi_{n'\mathbf{k}'} \psi_{n\mathbf{k}} d^3r = \delta_{n',n} \delta_{\mathbf{k}',\mathbf{k}} \quad (\text{A.8})$$

The wavefunctions are also normalized over the volume V of the crystal and therefore

$$\psi_{n\mathbf{k}} = V^{-1/2} U_{n\mathbf{k}}(r) \exp(j\mathbf{k} \cdot \mathbf{r}) \quad (\text{A.9})$$

A.2 The *k.p* Perturbation Theory Neglecting Spin

Complete knowledge of the band structure of a semiconductor requires that the full E - \mathbf{k} dispersion relation be known completely. The Schrödinger equation should therefore be solved completely. This is a rather difficult task since the form of the periodic potential $V(\mathbf{r})$ must be specified. Fortunately, in most descriptions of the electron and hole properties in semiconductors, the mostly populated electron and hole states lie within a fraction of an eV from the band edges. Thus, if the wavefunctions and energies of the carriers are known at the band extrema, then perturbation methods may be applied to find out the wavefunctions and energies at other points in the Brillouin zone, leading to knowledge of the E - \mathbf{k} relationship. The method, known as ***k.p** perturbation theory*, is most widely used in the study of transport and optical processes in common semiconductors [3–9].

The ***k.p*** perturbation theory is based on the fact that the cell periodic part $U_{\mathbf{k}}$ of the electrons, for any value of \mathbf{k} but different bands, forms a complete set. Let us consider the wavefunctions for the electrons having a value \mathbf{k} near the minima in the n th band. For simplicity we assume that the minima are located at $\mathbf{k} = 0$. The theory is applicable also when the minima are located at $\mathbf{k} = \mathbf{k}_0$. The wavefunction is given by

$$\psi = U_{n\mathbf{k}}(\mathbf{r}) \exp(j\mathbf{k} \cdot \mathbf{r}) = \left[\sum_m c_m U_{m0}(\mathbf{r}) \right] \exp(j\mathbf{k} \cdot \mathbf{r}), \quad (\text{A.10})$$

since U_{m0} forms a complete orthonormal set. Using this form of ψ in the Schrödinger equation, one obtains

$$\left[-\frac{\hbar^2}{2m_0} \nabla^2 + \frac{\hbar^2}{m_0} \mathbf{k} \cdot \mathbf{p} + \frac{\hbar^2 k^2}{2m_0} + V(\mathbf{r}) \right] U_{nk}(\mathbf{r}) = E_n(\mathbf{k}) U_{nk}(\mathbf{r}). \quad (\text{A.11})$$

However, U_{m0} is the wavefunction for $\mathbf{k} = 0$ in the n th band satisfying the equation

$$\left[-\frac{\hbar^2}{2m_0} \nabla^2 + V(\mathbf{r}) \right] U_{m0}(\mathbf{r}) = E_m(0) U_{m0}(\mathbf{r}). \quad (\text{A.12})$$

We now put Eq. (A.10) in (A.11) and use (A.12) to obtain

$$\sum_m c_m \left[E_m(0) + \frac{\hbar^2}{2m_0} k^2 + \frac{\hbar^2}{m_0} \mathbf{k} \cdot \mathbf{p} \right] U_{m0}(\mathbf{r}) = \sum_m c_m E_n(\mathbf{k}) U_{m0}(\mathbf{r}). \quad (\text{A.13})$$

Multiplying both sides of Eq. (A.13) by $U_{l0}^*(\mathbf{r})$ and integrating over a volume of a unit cell (V_c), the following set of linear homogeneous equations is obtained:

$$c_l \left[E_n(\mathbf{k}) - E_l(0) - \frac{\hbar^2}{2m_0} k^2 \right] - \sum_m c_m \frac{\hbar}{m_0} (\mathbf{k} \cdot \mathbf{p}_{lm}) = 0, \quad (\text{A.14})$$

where

$$\mathbf{p}_{lm} = \int_{V_c} U_{l0}^*(\mathbf{r}) \mathbf{p} U_{m0}(\mathbf{r}) d^3r. \quad (\text{A.15})$$

By giving l successive integer values, one obtains the full set of equations.

In the general case, the set of equations has a nontrivial solution if the determinant of the coefficients c_l is zero. This condition gives the energy eigenvalues $E_n(\mathbf{k})$ in terms of the quantities $E_m(0)$ and p_{lm} . The relative values of the expansion coefficients c_m are then obtained by using the values of $E_n(\mathbf{k})$. The absolute values of c_m are obtained by imposing normalization conditions on ψ . The accuracy of the calculation is increased if many such coefficients are included. For practical reasons we need to limit ourselves to a few bands. The bands of greatest interest in common semiconductors are conduction (C), heavy hole (HH), light hole (LH), and split-off (SO) bands. Each of these four bands has two spin components, so there are altogether eight bands. Depending on the problem at hand and the degree of accuracy required, we may use some or all of these eight bands. We present below the results by using different approximations regarding the number of bands.

A.2.1 Single-Electron Band

Let us assume that U_{nk} is determined mostly by U_{n0} and the contributions from other bands are smaller. In other words, we assume that $c_m(m \neq n) \ll c_n$. Then

$$\psi = \left[c_n U_{n0}(\mathbf{r}) + \sum_m c_m U_{m0}(\mathbf{r}) \right] \exp(j\mathbf{k} \cdot \mathbf{r}). \quad (\text{A.16})$$

Since ψ is normalized, $\sum_m |c_m|^2 = 1$; but we have assumed $c_m \ll c_n$. It follows, therefore, that $c_n \approx 1$.

To solve Eq. (A.16), stationary perturbation theory is applied. First, neglect c_m ($m \neq n$) in comparison to c_n in the n th equation. The result is

$$E_n(\mathbf{k}) = E_n(0) + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p}_{nn}. \quad (\text{A.17})$$

Next put $c_n = 1$ and obtain from Eq. (A.14)

$$c_m \approx \frac{\hbar}{m_0} \frac{\mathbf{k} \cdot \mathbf{p}_{mn}}{E_n(0) - E_m(0)} c_n, \quad (\text{A.18})$$

neglecting the $\mathbf{k} \cdot \mathbf{p}$ term in the denominator. If this expression for c_m is now used in Eq. (A.14), a second-order approximation results and one obtains

$$E_n(\mathbf{k}) = E_n(0) + \frac{\hbar^2 k^2}{2m_0} + \frac{\hbar}{m_0} \mathbf{k} \cdot \mathbf{p}_{nn} + \sum_{m \neq n} \left(\frac{\hbar}{m_0} \right)^2 \frac{|\mathbf{k} \cdot \mathbf{p}_{nm}|^2}{E_n(0) - E_m(0)}. \quad (\text{A.19})$$

Since the extrema occur at $\mathbf{k} = 0$, $\mathbf{p}_{nn} = 0$. Therefore, by choosing a proper coordinate system, one may write

$$E_n(\mathbf{k}) = E_n(0) + \frac{\hbar^2 k^2}{2m_i},$$

where, from Eq. (A.19),

$$\frac{1}{m_i} = \frac{1}{m_0} + \frac{2}{m_0^2} \sum_m \frac{|\mathbf{i} \cdot \mathbf{p}_{nm}|^2}{E_n(0) - E_m(0)}, \quad (\text{A.20})$$

where \mathbf{i} is a unit vector along the i th coordinate axis. The above equation predicts a parabolic E - \mathbf{k} relation.

The analysis presented in this subsection may be improved by combining with the band under consideration other bands close to it and treating the effects of the additional bands as small perturbations.

A.2.2 Four Bands

We now consider four bands: the C, HH, LH, and SO bands. The valence bands are triply degenerate, and the C-band minima and H-band maxima occur at $\mathbf{k} = 0$. For the present, the spin-orbit interaction is neglected. We denote the cell periodic parts of the conduction band by U_c and those of the three valence bands by U_{v1} , U_{v2} , U_{v3} . Also the symbols E_c and E_v are used to denote, respectively, the energy for conduction band minima and valence band maxima. We may write the wavefunction for any \mathbf{k} as

$$\psi = (a_k U_c + b_k U_{v1} + c_k U_{v3} + d_k U_{v2}) \exp(j\mathbf{k} \cdot \mathbf{r}), \quad (\text{A.21})$$

in accordance with Eq. (A.10). Using the symbol $E' = E - \hbar^2 k^2 / 2m_0$, the linear homogeneous equations are

$$\begin{aligned} a_k(E' - E_c) - (\hbar/m_0)\mathbf{k} \cdot (b_k \mathbf{p}_{cv1} + d_k \mathbf{p}_{cv2} + c_k \mathbf{p}_{cv3}) &= 0 \\ -a_k(\hbar/m_0)\mathbf{k} \cdot \mathbf{p}_{cv1} + b_k(E' - E_v) - (\hbar/m_0)\mathbf{k} \cdot (d_k \mathbf{p}_{v1v2} + c_k \mathbf{p}_{v1v3}) &= 0 \\ -a_k(\hbar/m_0)\mathbf{k} \cdot \mathbf{p}_{cv2} - b_k(\hbar/m_0)\mathbf{k} \cdot \mathbf{p}_{v1v2} - d_k(E' - E_v) - (\hbar/m_0)\mathbf{k} \cdot c_k &= 0 \\ -a_k(\hbar/m_0)\mathbf{k} \cdot \mathbf{p}_{cv3} - b_k(\hbar/m_0)\mathbf{k} \cdot \mathbf{p}_{v1v3} - d_k(\hbar/m_0)\mathbf{k} \cdot c_k + c_k(E' - E_v) &= 0 \end{aligned} \quad (\text{A.22})$$

The quantities p_{cv1} , p_{v1v2} , and so on are defined in Eq. (A.15). The matrix elements may be evaluated once the U_s are known. Since U_c is an atomic s -like function and the U_v 's are p -like functions, the $\mathbf{k} \cdot \mathbf{p}_{cv1}$ term may be expressed as

$$h_1 = \frac{\hbar^2}{m_0 j} \int U_t^* \left(k_x \frac{\partial}{\partial x} + k_y \frac{\partial}{\partial y} + k_z \frac{\partial}{\partial z} \right) U_m d^3 r \quad t, m = s, x, y, z. \quad (\text{A.23})$$

Since $(\partial/\partial x)U_s$ is an odd function of x , the matrix element $\int U_j^* (\partial/\partial x)U_s dx$ is nonzero only when $j = x$. The same is true for $\int U_s^* (\partial/\partial x)U_j dx$. The function $(\partial/\partial x)U_y$ is odd in both x and y . Thus

$$\iint U_j^* \frac{\partial}{\partial x} U_y dx dy = 0, \quad j = s, x, y, z.$$

The only nonvanishing matrix elements are the ones defined by the following expressions:

$$P = -\frac{\hbar^2}{m_0} \int U_j \frac{\partial}{\partial j} U_s d^3 r = -\frac{\hbar^2}{m_0} \int U_s \frac{\partial}{\partial j} U_j d^3 r, \quad j = x, y, z. \quad (\text{A.24})$$

In the following, we shall assume that \mathbf{k} is parallel to the z direction. Then we may rewrite the four homogeneous equations (A.22) as

$$\begin{aligned} a_k(E' - E_c) - c_k P k &= 0, \\ b_k(E' - E_v) &= 0, \\ -a_k P k c_k(E' - E_v) &= 0, \\ d_k(E' - E_v) &= 0. \end{aligned} \quad (\text{A.25})$$

The energy eigenvalues are thus given by

$$E' = E_c, E_v \text{ and } (E' - E_c)(E' - E_v) - P^2 k^2 = 0. \quad (\text{A.26})$$

These equations give the dispersion relations when the conduction bands and valence bands are strongly coupled. Denoting the energy gap by $E_g = E_c - E_v$, we may write Eq. (A.26) as

$$(E' - E_c)(E' - E_c + E_g) - P^2 k^2 = 0.$$

When E' tends to E_c , we may neglect $E' - E_c$ in comparison to E_g and write

$$(E' - E_c)E_g = P^2 k^2. \quad (\text{A.27})$$

If the band edge effective mass is denoted by m_{e0} , we obtain

$$P^2 = \left(\frac{E - E_c - \hbar^2 k^2}{2m_0} \right) \frac{E_g}{k^2} = \hbar^2 \left(\frac{1}{m_{e0}} - \frac{1}{m_0} \right) \frac{E_g}{2}. \quad (\text{A.28})$$

A.3 Spin–Orbit Interaction

The electron is a fermion with spin $1/2$ in units of \hbar . In classical mechanics, a point particle rotating about an axis has an angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. In the quantum picture, the angular momentum of a point particle is quantized and the intrinsic value of the momentum is called the *spin*. There is strong interaction between the spin and orbital motion of the electrons. This spin–orbit coupling may be calculated for isolated atoms; however, it is difficult to do so in crystals.

A.3.1 Spin–Orbit Interaction Term

To calculate the interaction a general form of spin–orbit interaction is assumed with a fitting parameter that is adjusted to fit experimentally observed effects. The total Hamiltonian in the presence of spin–orbit interaction is written as $H = H_0 + H_{so}$, where H_0 is the Hamiltonian without interaction and H_{so} is the spin–orbit interaction written as

$$H_{so} = \lambda \mathbf{L} \cdot \mathbf{S}. \quad (\text{A.29})$$

Here \mathbf{L} represents the operator for orbital angular momentum, \mathbf{S} is the operator for spin angular momentum, and λ is treated as a constant. The total angular momentum \mathbf{J} may be expressed as

$$\mathbf{J}^2 = (\mathbf{L} + \mathbf{S})^2 = L^2 + S^2 + 2\mathbf{L} \cdot \mathbf{S}. \quad (\text{A.30a})$$

Thus

$$\langle \mathbf{L} \cdot \mathbf{S} \rangle = (1/2) \langle J^2 - L^2 - S^2 \rangle = \frac{\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)], \quad (\text{A.30b})$$

where j , l , and s are the quantum numbers for the operators \mathbf{J} , \mathbf{L} , and \mathbf{S} , respectively. However, to calculate the spin–orbit interaction energy, one needs the pure angular momentum states to which Eq. (A.30) is applicable. One should note that states like $|X\alpha\rangle$ are mixed states, with the symbol α denoting the spin-up state. To illustrate this statement, we express $|X\rangle$ in terms of pure angular momentum states, that is,

$$\begin{aligned} |X\rangle &= \frac{1}{\sqrt{2}} (-\phi_{1,1} + \phi_{1,-1}) \\ |Y\rangle &= \frac{j}{\sqrt{2}} (\phi_{1,1} + \phi_{1,-1}) \\ |Z\rangle &= \phi_{1,0} \end{aligned} \quad (\text{A.31})$$

The ϕ_{ij} 's are pure angular momentum states, and the expressions for the lower eigenstates are

$$\begin{aligned} \phi_{1,\pm 1} &= Y_{1,\pm 1}(\theta, \phi) = \mp \sqrt{\frac{3}{8\pi}} \sin \theta \exp(\pm j\phi) \\ \phi_{1,0} &= Y_{1,0}(\theta, \phi) = \sqrt{\frac{3}{4\pi}} \cos \theta \end{aligned}$$

The ϕ_{ij} 's are eigenfunctions of L^2 and L_z . The respective quantum numbers are $l = I$ and $l_z = j$. For example, $L^2\phi_{1,-1} = \hbar^2(1)(1+1)\phi_{1,-1} = 2\hbar^2\phi_{1,-1}$ and $L_z\phi_{1,-1} = -1\hbar\phi_{1,-1}$.

Equation (A.31) is modified if spin is included; for example, the spin-up state $p_x = |X\alpha\rangle$ is expressed as

$$|X\alpha\rangle = \frac{1}{\sqrt{2}}(-\phi_{1,1} + \phi_{1,-1})\alpha.$$

This formulation is still in terms of mixed states. To decompose the mixed states into states of pure angular momentum, the spin and orbital angular momentum must be added to obtain the total angular momentum states. The standard Clebsch–Gordan (CG) technique is employed for this addition. The following six equations are obtained as a result:

$$\begin{aligned}\phi_{3/2,3/2} &= \phi_{1,1}\alpha = (-1/\sqrt{2})|(X+jY)\alpha\rangle \\ \phi_{3/2,1/2} &= \frac{1}{\sqrt{3}}\phi_{1,1}\beta + \frac{2}{\sqrt{6}}\phi_{1,0}\alpha = \frac{-1}{\sqrt{6}}[|(X+jY)\beta\rangle - |2Z\alpha\rangle] \\ \phi_{3/2,-1/2} &= \frac{1}{6}\phi_{1,0}\beta + \frac{1}{\sqrt{3}}\phi_{1,-1}\alpha = \frac{1}{\sqrt{6}}[|(X-jY)\alpha\rangle + |2Z\beta\rangle] \\ \phi_{3/2,-3/2} &= \phi_{1,-1}\beta = (1/\sqrt{2})|(X-jY)\beta\rangle \\ \phi_{1/2,1/2} &= \frac{-1}{\sqrt{3}}\phi_{1,0}\alpha + \frac{2}{\sqrt{6}}\phi_{1,1}\beta = \frac{-1}{\sqrt{3}}[|(X+jY)\beta\rangle + |Z\alpha\rangle] \\ \phi_{1/2,-1/2} &= \frac{-2}{\sqrt{6}}\phi_{1,-1}\alpha + \frac{1}{\sqrt{3}}\phi_{1,0}\beta = \frac{-1}{\sqrt{3}}[|(X-jY)\alpha\rangle - |Z\beta\rangle]\end{aligned}\tag{A.32}$$

These six equations are inverted to find states like $\phi_{1,0}$, and from the resultant equations one gets states like $|X\alpha\rangle$, and so on.

$$\begin{aligned}|X\alpha\rangle &= \frac{1}{\sqrt{2}}\left[-\phi_{3/2,3/2} + \frac{1}{\sqrt{3}}\phi_{3/2,-1/2} - \sqrt{\frac{2}{3}}\phi_{1/2,-1/2}\right] \\ |X\beta\rangle &= \frac{1}{\sqrt{2}}\left[-\frac{1}{\sqrt{3}}\phi_{3/2,1/2} - \frac{2}{\sqrt{3}}\phi_{1/2,1/2} - \phi_{3/2,-3/2}\right] \\ |Y\alpha\rangle &= \frac{j}{\sqrt{2}}\left[\phi_{3/2,3/2} + \frac{1}{\sqrt{3}}\phi_{3/2,-1/2} - \sqrt{\frac{2}{3}}\phi_{1/2,-1/2}\right] \\ |Y\beta\rangle &= \frac{j}{\sqrt{2}}\left[\frac{1}{\sqrt{3}}\phi_{3/2,1/2} + \frac{2}{\sqrt{3}}\phi_{1/2,1/2} + \phi_{3/2,-3/2}\right] \\ |Z\alpha\rangle &= \sqrt{\frac{2}{3}}\phi_{3/2,1/2} - \frac{1}{\sqrt{3}}\phi_{1/2,1/2} \\ |Z\beta\rangle &= \sqrt{\frac{2}{3}}\phi_{3/2,-1/2} + \frac{1}{\sqrt{3}}\phi_{1/2,-1/2}.\end{aligned}\tag{A.33}$$

The phases used in the above expressions for ϕ_{j,m_j} in terms of $|X\alpha\rangle, \dots, |Z\beta\rangle$ are obtained in the standard derivation of Clebsch–Gordan coefficients. The overall phase of a state is

arbitrary and has no effect on the physical predictions. The convention used by Luttinger and Kohn [10] is in widespread use and will be used here. The states are expressed in terms of CG states as

$$\begin{aligned}
 \phi_{3/2,3/2}(\text{LK}) &= -\phi_{3/2,3/2}(\text{CG}) = \frac{1}{\sqrt{2}}|(X+jY)\alpha\rangle \\
 \phi_{3/2,1/2}(\text{LK}) &= -j\phi_{3/2,1/2}(\text{CG}) \\
 \phi_{3/2,-1/2}(\text{LK}) &= \phi_{3/2,-1/2}(\text{CG}) \\
 \phi_{3/2,-3/2}(\text{LK}) &= j\phi_{3/2,-3/2}(\text{CG}) \\
 \phi_{1/2,1/2}(\text{LK}) &= -\phi_{1/2,1/2}(\text{CG}) \\
 \phi_{1/2,-1/2}(\text{LK}) &= j\phi_{1/2,-1/2}(\text{CG})
 \end{aligned} \tag{A.34}$$

The spin-orbit Hamiltonian may be calculated now with the above states. The interaction is

$$H_{so} = \frac{\lambda\hbar^2}{2} [j(j+1) - l(l+1) - s(s+1)] \tag{A.35}$$

For p-type electron orbitals $l=1$ and $s=1/2$, j is given by the first subscript of ϕ in Eq. (A.33). Many terms become zero as the pure states are orthogonal. We conclude that only the following terms are nonzero:

$$\begin{aligned}
 \langle X\alpha|H_{so}|Y\alpha\rangle &= \langle Y\alpha|H_{so}|Z\beta\rangle = \langle Y\beta|H_{so}|Z\alpha\rangle = -j\frac{\Delta}{3} \\
 \langle X\alpha|H_{so}|Z\beta\rangle &= \frac{\Delta}{3}; \quad \langle X\beta|H_{so}|Z\alpha\rangle = -\frac{\Delta}{3}; \quad \langle X\beta|H_{so}|Y\beta\rangle = j\frac{\Delta}{3},
 \end{aligned} \tag{A.36}$$

where Δ is a parameter known as *spin-orbit splitting* given by $\Delta = \Delta_{so} = 3\lambda\hbar^2/2$.

A.3.2 Conduction Band Energy

The calculation of energy levels in the conduction band by including the spin-orbit interaction is easier, and therefore we consider it first. As mentioned previously, we are interested in four basic vectors, the $|S\rangle$ state for the conduction band and the $|X\rangle, |Y\rangle, |Z\rangle$ states for the valence bands. There are four coefficients, $a_k \dots d_k$ as in Eq. (A.21), needed to describe a state. With the inclusion of spin, the number of basis vectors to be considered becomes eight. The secular equation containing the coefficients and basis vectors involves an 8×8 matrix. It turns out that if the basis vectors are arranged in the following manner,

$$|S\alpha\rangle, |(X+jY)\beta\rangle, |Z\alpha\rangle, |(X-jY)\beta\rangle, |S\beta\rangle, |(X-jY)\alpha\rangle, |Z\beta\rangle, \text{ and } |-(X+jY)\alpha\rangle,$$

the matrix may be written in the form

$$\begin{bmatrix} H & 0 \\ 0 & H \end{bmatrix},$$

where H is a 4×4 matrix. Using the matrix elements between different states and the earlier elements obtained without the spin-orbit interactions, we may express the different

matrix elements in terms of P in the following form:

$$\begin{array}{ccccc}
 & |S\alpha\rangle & |(X+jY)\beta\rangle & |Z\alpha\rangle & |(X-jY)\beta\rangle \\
 |S\alpha\rangle & E_s - E' & 0 & -jkP & 0 \\
 |(X+jY)\beta\rangle & 0 & E_p - E' - \Delta/3 & \sqrt{2}\Delta/3 & 0 \\
 |Z\alpha\rangle & jkP & \sqrt{2}\Delta/3 & E_p - E' & 0 \\
 |(X-jY)\beta\rangle & 0 & 0 & 0 & E_p - E' + \Delta/3
 \end{array} \quad (A.37)$$

To simplify the calculation, we choose the k -vector in (A.37) along the z -direction. Furthermore, to account for the shift of band energies due to spin-orbit interaction, notations E_p and E_s are used. The difference in signs in $E_p - E' \pm \Delta/3$ is due to the fact that $L_z S_z |(X+jY)\beta\rangle = -|(X+jY)\beta\rangle$ while $L_z S_z |(X-jY)\beta\rangle = |(X-jY)\beta\rangle$. Expanding (A.37) one obtains

$$E' = E_p + \Delta/3 \quad (A.38a)$$

$$\left(E' - E_p + \frac{2\Delta}{3}\right) \left(E' - E_p - \frac{\Delta}{3}\right) (E' - E_s) - k^2 P^2 \left(E' - E_p + \frac{\Delta}{3}\right) = 0 \quad (A.38b)$$

For small values of k^2 , the cubic equation can easily be solved by treating the term $k^2 P^2$ as a small perturbation. This yields

$$E'_1 = E_s + \frac{k^2 P^2 (E_s - E_p + \Delta/3)}{(E_s - E_p + 2\Delta/3)(E_s - E_p - \Delta/3)}. \quad (A.38c)$$

Let $E_v = E_p + \Delta/3 = 0$, $E_c = E_s = E_{g0}$ and $E_c - E_v = E_{g0}$, the direct gap. We then rewrite Eq. (A.38a) as

$$E'(E' - E_{g0})(E' + \Delta) - k^2 P^2 (E' + 2\Delta/3) = 0. \quad (A.39)$$

Taking $E_c = E_{g0}$ in the first approximation,

$$E_c(\mathbf{k}) = E_{g0} + \frac{\hbar^2 k^2}{2m_0} + \frac{k^2 P^2}{3} \left[\frac{2}{E_{g0}} + \frac{1}{E_{g0} + \Delta} \right]. \quad (A.40a)$$

We also obtain, by putting $E_v = E_p + \Delta/3 = 0$,

$$E_{v1}(\mathbf{k}) = \frac{\hbar^2 k^2}{2m_0}. \quad (A.40b)$$

Taking $E = 0$,

$$E_{v2} = \frac{\hbar^2 k^2}{2m_0} - \frac{2k^2 P^2}{3E_{g0}}. \quad (A.40c)$$

Finally, taking $E' = -\Delta$ as a first approximation,

$$E_{v3} = -\Delta + \frac{\hbar^2 k^2}{2m_0} - \frac{k^2 P^2}{3(E_{g0} + \Delta)}. \quad (A.40d)$$

In Eq. (A.40a), E_c is the energy of the conduction band electrons, while E_{v1} , E_{v2} , and E_{v3} , are, respectively, the energies of the three valence bands. From Eq. (A.40a), we may define the band edge effective mass for conduction band electrons by writing

$$E_c = E_{g0} + \hbar^2 k^2 / 2m_{e0}.$$

It then follows that

$$\frac{1}{m_{e0}} = \frac{1}{m_0} + \frac{2P^2}{3\hbar^2} \left(\frac{2}{E_{g0}} + \frac{1}{E_{g0} + \Delta} \right). \quad (\text{A.41})$$

The momentum matrix element, P , which is central to all calculation of transition probabilities from the valence band to the conduction band, may be expressed in terms of m_{e0} as

$$P^2 = \frac{\hbar^2}{2m_{e0}} \frac{E_{g0}(E_{g0} + \Delta)}{E_{g0} + 2\Delta/3} \frac{m_0 - m_{e0}}{m_0}. \quad (\text{A.42})$$

A.3.3 Valence Band Energies

The earlier treatment of the dispersion relation cannot explain the properties of electrons in the valence band. Referring to Eq. (A.40a), one notices that the energy of the electrons increases with k , which however is opposite to what is observed experimentally. To treat the valence band properties correctly, degenerate perturbation theory is needed [11].

Let the state of the electron in the l th band at $k=0$ be degenerate, having f -fold degeneracy. It follows from the theory of perturbation of degenerate states that the second-order corrections $\Delta E^{(2)}$ due to the $(\hbar/m_0)(\mathbf{k} \cdot \mathbf{p})$ perturbation are the roots of the secular equation

$$\left[\left(\frac{\hbar^2}{m_0} \right)^2 \sum_{n,s}' \frac{\langle l, r' | \mathbf{k} \cdot \mathbf{p} | n, s \rangle \langle n, s | \mathbf{k} \cdot \mathbf{p} | l, r \rangle}{E_l(0) - E_n(0)} - \Delta E^{(2)} \delta_{rr'} \right] = 0, \quad (\text{A.43})$$

where the primed summation sign indicates that the summation is over all $n \neq l$ and over $s, |l, r\rangle$ and $|l, r'\rangle$ are the unperturbed f -fold degenerate wavefunctions ($r, r' = 1, 2, \dots, f$) satisfying Eq. (A.43) for the energy eigenvalue $E_l(0)$. The $|n, s\rangle$'s are the wavefunctions for energy level $E_n(0)$. The order of the determinant of the secular equation is equal to the degree of degeneracy of the level $E_l(0)$. In the present situation, the degenerate eigenstates at $k=0$ are the three $l=1, m_l=0$, and ± 1 states. To the second order in perturbation, the energy in the n th band is

$$E_n(k) = E_n(0) + \frac{\hbar^2 k^2}{2m_0} + \Delta E_n^{(2)}(k), \quad (\text{A.44})$$

where $\Delta E_n^{(2)}$ is given by Eq. (A.43) above. Hence we have the set of three equations

$$\sum_{i=1}^3 \left[\sum_m' \frac{\langle j|H_l|m\rangle \langle m|H_l|l\rangle}{E_l(0) - E_m(0)} + \left\{ E_l + \frac{\hbar^2 k^2}{2m_0} - E_n(k) \right\} \delta_{j,l} \right] \langle n|k\rangle = 0. \quad (\text{A.45})$$

Nontrivial solutions of this set of N coupled homogeneous equations occur only if

$$\det[|H| - E_n(k)\mathbf{I}] = 0,$$

where \mathbf{I} is the identity matrix and H is a 3×3 matrix whose elements are

$$H_{jl} = \left[E_l + \frac{\hbar^2 k^2}{2m_0} \right] \delta_{jl} + \sum_m' \frac{\langle j|H_l|m\rangle \langle m|H_l|l\rangle}{E_l(0) - E_m(0)}.$$

The calculation of the matrix element is first made by ignoring the spin-orbit interaction for the present. We take the basis sets as $|X\rangle, |Y\rangle$ and $|Z\rangle$. Then

$$H_{11} = \langle X|H|X\rangle = E_1(0) + \frac{\hbar^2 k^2}{2m_0} + \sum_m' \frac{|\langle X|H_l|m\rangle|^2}{E_l(0) - E_m(0)}. \quad (\text{A.46})$$

Since $|X\rangle$ is proportional to $x f(\mathbf{r})$, we may verify that

$$\frac{m_0^2}{\hbar^2} |\langle X|H_l|m\rangle|^2 = |\langle X|p_x|m\rangle|^2 k_x^2 + |\langle X|p_y|m\rangle|^2 k_y^2 + |\langle X|p_z|m\rangle|^2 k_z^2.$$

Thus we may write

$$H_{11} = E_1 + \sum_{j=x,y,z} \left[\frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0^2} \sum_m' \frac{|\langle X|p_j|m\rangle|^2}{E_l - E_m} \right] k_j^2.$$

Due to symmetry at $k=0$,

$$|\langle X|p_y|m\rangle|^2 = |\langle X|p_z|m\rangle|^2.$$

Therefore,

$$H_{11} = E_1 + A k_x^2 + B(k_y^2 + k_z^2), \quad (\text{A.47a})$$

where

$$A = \frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0^2} \sum_j' \frac{|\langle X|p_x|j\rangle|^2}{E_l - E_j}, \quad (\text{A.47b})$$

$$B = \frac{\hbar^2}{2m_0} + \frac{\hbar^2}{m_0^2} \sum_j' \frac{|\langle X|p_y|j\rangle|^2}{E_l - E_j}. \quad (\text{A.47c})$$

The remaining matrix elements can be evaluated in a similar way to give the following Hamiltonian matrix,

$$H = \begin{bmatrix} E_1 + Ak_x^2 + B(k_y^2 + k_z^2) & Ck_xk_y & Ck_xk_z \\ Ck_xk_y & E_1 + Ak_y^2 + B(k_x^2 + k_z^2) & Ck_yk_z \\ Ck_xk_z & Ck_yk_z & E_1 + Ak_z^2 + B(k_x^2 + k_y^2) \end{bmatrix} \quad (\text{A.48})$$

where

$$C = \frac{\hbar^2}{m_0^2} \sum_j \frac{\langle X|p_x|j\rangle\langle j|p_y|Y\rangle + \langle X|p_y|j\rangle\langle j|p_x|Y\rangle}{E_l - E_j}. \quad (\text{A.49})$$

Let us now consider the effect of spin. As noted earlier in Eq. (A.30) for $j = 1/2$, $\langle \mathbf{L} \cdot \mathbf{S} \rangle = -\hbar^2$, and for $j = 3/2$, $\langle \mathbf{L} \cdot \mathbf{S} \rangle = +\hbar^2/2$. Thus the states are split by an amount Δ proportional to $(3/2)\hbar^2$, the doubly degenerate state with $j = 3/2$ moving up by $\Delta/3$ and the single $j = 1/2$ state moving down by $2\Delta/3$. Since in the designation $|ls; jm_j\rangle$, $l = 1$ and $s = 1/2$, we shall use only the symbol $|jm_j\rangle$ to denote the states. As noted in this appendix, the Hamiltonian for the spin-orbit coupling is diagonalized if the states are chosen according to Eq. (A.32).

We shall treat the $j = 3/2$ states and $j = 1/2$ states separately, since the splitting energy is large. The Hamiltonian matrix $|H|$ now becomes a 4×4 matrix for $j = 3/2$ states and a 2×2 matrix for $j = 1/2$ states. We may evaluate the matrix elements for the 4×4 matrix using Eq. (A.47). Thus

$$\begin{aligned} H_{11} &= \langle 3/2, 3/2 | H | 3/2, 3/2 \rangle = (1/2) \langle (X + jY)\alpha | H | (X + jY)\alpha \rangle \\ &= (1/2) [\langle X\alpha | H | X\alpha \rangle + \langle Y\alpha | H | Y\alpha \rangle + j \langle X\alpha | H | Y\alpha \rangle - j \langle Y\alpha | H | X\alpha \rangle] \\ &= E_1 + \frac{A}{2} (k_x^2 + k_y^2) + \frac{B}{2} (k_x^2 + k_y^2 + 2k_z^2) \\ &= H_{44} \end{aligned} \quad (\text{A.50})$$

where the symbols 1, 2, 3, and 4 are used in the order in which the states are written in Eq. (A.48). Similarly,

$$H_{12} = \frac{1}{2\sqrt{3}} \langle (X + jY)\alpha | H | [(X + jY)\beta - 2Z\alpha] \rangle = \frac{1}{\sqrt{3}} (H_{xz} - jH_{yz}).$$

Instead of computing matrix elements $\langle n|p|m\rangle$ from first principles, one replaces them with experimentally determined parameters called *Luttinger parameters*, defined as

$$\gamma_1 = -2m_0(A + 2B)/3\hbar^2, \quad \gamma_2 = -m_0(A - B)/3\hbar^2, \quad \gamma_3 = -m_0C/3\hbar^2. \quad (\text{A.51})$$

In terms of Luttinger parameters,

$$H_{11} = E_1 - \frac{\hbar^2 k_z^2}{2m_0} (\gamma_1 - 2\gamma_2) - \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_0} (\gamma_1 + \gamma_2) \quad (\text{A.52})$$

Since in measurements the parameters conform to holes, and since the hole energy is positive, we write $H_{11} = -H_{hh}$ and the zero energy reference is $E_1 = 0$. Repeating the above

calculation for the other matrix elements, we obtain for the Luttinger Hamiltonian,

$$H = \begin{bmatrix} H_{hh} & -c & -b & 0 \\ -c^* & H_{lh} & 0 & b \\ -b^* & 0 & H_{lh} & -c \\ 0 & b^* & -c^* & H_{hh} \end{bmatrix} \quad (\text{A.53})$$

where

$$\begin{aligned} H_{lh} &= \frac{\hbar^2 k_z^2}{2m_0} (\gamma_1 + 2\gamma_2) - \frac{\hbar^2 (k_x^2 + k_y^2)}{2m_0} (\gamma_1 - \gamma_2) \\ c &= \frac{\sqrt{3}\hbar^2}{2m_0} \left[\gamma_2 (k_x^2 - k_y^2) - 2j\gamma_3 k_x k_y \right] \\ b &= \frac{\sqrt{3}\hbar^2}{m_0} \gamma_3 k_z (k_x - jk_y). \end{aligned} \quad (\text{A.54})$$

In the vicinity of $k = 0$, one may use the axial approximation, where γ_2 and γ_3 are replaced by an effective Luttinger parameter,

$$\bar{\gamma} = (1/2)(\gamma_2 + \gamma_3) \quad (\text{A.55})$$

The function c is then expressed as

$$c \cong \frac{\sqrt{3}\hbar^2 \bar{\gamma}}{2m_0} (k_x - jk_y)^2 \quad (\text{A.56})$$

The dispersion relation for valence band holes may be written as

$$\begin{aligned} E_v &= -\frac{\hbar^2}{2m_0} \left[Ak^2 \pm \left\{ B^2 k^4 + C^2 (k_x^2 k_y^2 + k_x^2 k_z^2 + k_y^2 k_z^2) \right\}^{1/2} \right] \\ &= \frac{\hbar^2}{2m_0} \left[-\gamma_1 k^2 \pm \left\{ 4\gamma_2^2 k^4 + 12(\gamma_3^2 - \gamma_2^2) (k_x^2 k_y^2 + k_x^2 k_z^2 + k_y^2 k_z^2) \right\}^{1/2} \right] \end{aligned} \quad (\text{A.57})$$

Introducing the spherical polar coordinate system with the polar axis along the z -direction, we obtain

$$E_v = \frac{\hbar^2 k^2}{2m_0} \left[A \pm (B^2 + C^2/5)^{1/2} \right].$$

This enables us to define effective masses for heavy and light holes as

$$m_{hh} = \frac{m_0}{A - (B^2 + C^2/5)^{1/2}} \quad (\text{A.58a})$$

$$m_{lh} = \frac{m_0}{A + (B^2 + C^2/5)^{1/2}} \quad (\text{A.58b})$$

Example A.1

Using the values of γ 's in Table A.1, the band edge effective masses for Ge are $m_{hh} = 0.33 m_0$ and $m_{lh} = 0.04 m_0$; the values for Si are $m_{hh} = 0.56 m_0$ and $m_{lh} = 0.16 m_0$. For GaAs, the values are $m_{hh} = 0.059 m_0$ and $m_{lh} = 0.08 m_0$.

Table A.1 Band structure parameters for Ge, Si, and GaAs

	m_e/m_0	γ_1	γ_2	γ_3
Ge	1.58/0.082	13.25	4.20	5.56
Si	0.916/0.191	4.26	0.34	1.45
GaAs	0.067	6.8	2.1	2.9

A.3.4 Momentum Matrix Elements

It follows from Eq. (A.41) that the conduction band effective mass is expressed in terms of P and is related to p_{cv} , the momentum matrix element. The momentum matrix element also appears in the calculation of the optical absorption coefficient or the recombination rate in semiconductors. The conduction band edge state for a direct-gap semiconductor has been found to have *s*-type symmetry and is denoted by $|S\alpha\rangle$ and $|-S\beta\rangle$. The valence band states are written in terms of angular momentum spin representation in Eq. (A.32).

From symmetry, we find that only the matrix elements of the form

$$\langle X|p_x|S\rangle = \langle Y|p_y|S\rangle = \langle Z|p_z|S\rangle$$

are nonzero. The nonvanishing matrix elements are

$$\begin{aligned} \langle \pm 3/2|p_x|\pm S\rangle &= (1/\sqrt{2})\langle X|p_x|S\rangle, & \langle \pm 1/2|p_x|\mp S\rangle &= (1/\sqrt{6})\langle X|p_x|S\rangle \\ \langle \pm 3/2|p_x|\pm S\rangle &= (2/\sqrt{6})\langle X|p_x|S\rangle \end{aligned}$$

One may define a quantity:

$$E_p = \frac{2}{m_0} |\langle X|p_x|S\rangle|^2 = \frac{2}{m_0} p_{cv}^2$$

The values of E_p for different semiconductors are remarkably close to ~ 25 eV.

A.4 Quantum Wells

The subband structures for electrons and holes have been calculated in Chapter 3 by using simple theory. However, for refined calculation, complete knowledge of the E - \mathbf{k} dispersion relation is needed in order to explain the experimental results. Here we shall give the outline of the theory for valence band states in a quantum well.

A.4.1 Subband Structures for Holes

The degenerate nature of the valence bands prompts us to employ the multiband effective mass approximation. The Hamiltonian is written as

$$\sum_{v'} [H_{vv'}(\mathbf{k}) + V(z)\delta_{vv'}] \phi_m^{v'} = E_m \phi_m^v. \quad (\text{A.59})$$

The complete wavefunction for the valence band hole in the m th subband in the v th valence band $\varphi_{mk}(\mathbf{r})$ is written in terms of the envelope function ϕ_m^v as

$$\varphi_{mk}(r) = \sum_{v=1}^4 \phi_m^v(\mathbf{k}, z) \exp(j\mathbf{k} \cdot \mathbf{r}) U^v(\mathbf{r}). \quad (\text{A.60})$$

We have assumed as before that the conduction band is decoupled from the valence bands and only the two top valence bands are considered. We therefore consider four eigenstates: $|1\rangle = |3/2, 3/2\rangle$, $|2\rangle = |3/2, -1/2\rangle$, $|3\rangle = |3/2, 1/2\rangle$, $|4\rangle = |3/2, -3/2\rangle$.

The Luttinger Hamiltonians for the hole states are given by Eq. (A.53) and the coefficients are given in Eq. (A.54).

For a rectangular QW, $H_{vv'}(\mathbf{k})$ given in the matrix form described here should be replaced by $H_{vv'}(\mathbf{k}, -j\partial/\partial z)$, where \mathbf{k} is now the in-plane wave vector. The simple solution for $\mathbf{k} = 0$ has been worked out in Chapter 3 (see Eq. (3.57)).

The in-plane effective masses for holes in different subbands have been calculated by different authors using various degrees of approximations. We assume that the band gap as well as the separation between the heavy-hole and split-off bands are large, so that the Hamiltonian matrix is treated as a 4×4 matrix as before. The eigenvalues are obtained by solving the secular determinant of the 4×4 matrix, and the expression is given by (A.57).

The upper and lower signs correspond, respectively, to heavy- and light-hole bands. The character of the bands becomes increasingly mixed for higher values of \mathbf{k} . The effective mass in the xy plane depends, in general, on the direction, and the magnitude of the anisotropy is determined by the difference in γ_2 and γ_3 . In many cases the difference is small and it is justified to take a spherical average. It can be shown that the average $\langle k_x^2 k_y^2 + k_y^2 k_z^2 + k_z^2 k_x^2 \rangle \cong k^4/5$. Putting this in Eq. (A.57), we obtain

$$E = \frac{\hbar^2}{2m_0} (-\gamma_1 \pm 2\bar{\gamma}) k^2 \quad (\text{A.61})$$

where

$$\bar{\gamma}^2 = (2\gamma_2^2 + 3\gamma_3^2)/5. \quad (\text{A.62})$$

Each of the four eigenfunctions is of the form:

$$\varphi = [A|3/2, 3/2\rangle + B|3/2, -1/2\rangle + C|3/2, 1/2\rangle + D|3/2, -3/2\rangle] \exp(j\mathbf{k} \cdot \mathbf{r}) \quad (\text{A.63})$$

The four eigenfunctions may be expressed as column matrices.

In the practical situation when the barrier height is finite, a parameter $\bar{\gamma} = (\gamma_2 + \gamma_3)/2$ is introduced. The 4×4 Hamiltonian matrix is transformed to a new matrix \bar{H} by using a unitary matrix U such that [12]

$$\bar{H} = UH U^\dagger = \begin{bmatrix} H^U & 0 \\ 0 & H^L \end{bmatrix}, \quad (\text{A.64})$$

where

$$H^U = \begin{bmatrix} H_{hh} & R \\ R^* & H_{hh} \end{bmatrix} \quad \text{and} \quad H^L = \begin{bmatrix} H_{lh} & R \\ R^* & H_{lh} \end{bmatrix} \quad (\text{A.65})$$

$$R = |c| - j|b|$$

The upper and lower blocks are then decoupled. We write now the upper- and lower-block envelope functions as

$$\phi_{mk}^U(\mathbf{r}) = \sum_{v=1,2} g_m^{(v)}(\mathbf{k}, z) \exp(j\mathbf{k} \cdot \mathbf{r}) |v\rangle \quad (\text{A.66a})$$

and

$$\phi_{mk}^L(\mathbf{r}) = \sum_{v=2,4} g_m^{(v)}(\mathbf{k}, z) \exp(j\mathbf{k} \cdot \mathbf{r}) |v\rangle, \quad (\text{A.66b})$$

where $\{|v\rangle\}$ denotes the transformed basis set, and the envelope functions satisfy

$$\sum_{v'=1,2} \left[H_{vv'}^L \left(\mathbf{k}, -j \frac{\partial}{\partial z} \right) + V(z) \delta_{vv'} \right] g_m^{(v'+2)}(\mathbf{k}, z) = E_m^L(\mathbf{k}) g_m^{(v+2)}(\mathbf{k}, z). \quad (\text{A.67})$$

A.4.2 Subband Structures for Strained Ge on GeSiSn

The theoretical calculation by Chang and Chuang [13] is somewhat along the lines shown, but includes the strain effect. The upper- and lower-block Hamiltonians are expressed as

$$H_U = \begin{bmatrix} V_v(z) - P - Q & \bar{R} \\ \dot{R}^+ & V_v(z) - P + Q + \Delta Q \end{bmatrix} \quad (\text{A.68a})$$

$$H_L = \begin{bmatrix} V_v(z) - P + Q + \Delta Q & \bar{R} \\ \bar{R}^+ & V_v(z) - P - Q \end{bmatrix} \quad (\text{A.68b})$$

$$P = -\frac{\hbar^2}{2m_0} \frac{\partial}{\partial z} \gamma_1 \frac{\partial}{\partial z} + \frac{\gamma_1 \hbar^2 k_t^2}{2m_0} + P_\varepsilon$$

$$P_\varepsilon = -a_v(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$Q = \frac{\hbar^2}{2m_0} \frac{\partial}{\partial z} \gamma_2 \frac{\partial}{\partial z} + \frac{\gamma_2 \hbar^2 k_t^2}{2m_0} + Q_\varepsilon$$

$$Q_\varepsilon = -\frac{b_v}{2}(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})$$

$$\Delta Q = \frac{1}{2} \left[\sqrt{(\Delta + Q_\varepsilon)^2 + 8Q_\varepsilon^2} - (\Delta + Q_\varepsilon) \right]$$

$$\bar{R} = \frac{\sqrt{3}\hbar^2}{2m_0} \left[\left(\frac{\gamma_2 + \gamma_3}{2} \right) k_t^2 - k_t \left(\frac{\partial}{\partial z} \gamma_3 + \gamma_3 \frac{\partial}{\partial z} \right) \right]$$

$$\bar{R}^+ = \frac{\sqrt{3}\hbar^2}{2m_0} \left[\left(\frac{\gamma_2 + \gamma_3}{2} \right) k_t^2 + k_t \left(\frac{\partial}{\partial z} \gamma_3 + \gamma_3 \frac{\partial}{\partial z} \right) \right].$$

The symbols have their usual meanings.

In a QW grown along the [100] plane, all four L valleys are equivalent. The Hamiltonian for the [111] L valley may be written as

$$H_L^{[111]} \left(k_t, k_z = -j \frac{\partial}{\partial z} \right) - \frac{\hbar^2}{2} \frac{\partial}{\partial z} \left(\frac{1}{3m_l} + \frac{2}{3m_t} \right) \frac{\partial}{\partial z} - j \frac{\sqrt{2}\hbar^2 k_1}{6} \\ \times \left[\frac{\partial}{\partial z} \left(\frac{1}{m_l} - \frac{1}{m_t} \right) + \left(\frac{1}{m_l} - \frac{1}{m_t} \right) \frac{\partial}{\partial z} + \left(\frac{2}{3m_l} + \frac{1}{3m_t} \right) \frac{\hbar^2 k_1^2}{2} \right] \\ + \frac{\hbar^2 k_2^2}{2m_t} + V^{[111]}(z) + V_\varepsilon^{[111]}(z) \quad (\text{A.69})$$

$$V_\varepsilon^{[111]}(z) = a_L(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}) \\ k_1 = \frac{1}{\sqrt{2}} \left(k_x + k_y - \frac{2\pi}{a} \right) \\ k_2 = \frac{1}{\sqrt{2}} (-k_x + k_y)$$

A.4.3 Expression for Gain

In order to calculate the gain spectra, one needs to evaluate the squared momentum matrix elements for transverse electric (TE) and transverse magnetic (TM) configurations. We quote here the results for the TE momentum matrix element as given in Chang and Chuang.

$$M_{nm}^{U,TE}(k_t) = \frac{3}{2} \left| \int_{-\infty}^{\infty} dz \phi^*_{n,k_t=0}(z) M_b g_m^{(1)}(k_t, z) \right|^2 + \frac{1}{2} \left| \int_{-\infty}^{\infty} dz \phi^*_{n,k_t=0}(z) M_b g_m^{(2)}(k_t, z) \right|^2 \\ M_{nm}^{L,TE}(k_t) = \frac{3}{2} \left| \int_{-\infty}^{\infty} dz \phi^*_{n,k_t=0}(z) M_b g_m^{(4)}(k_t, z) \right|^2 + \frac{1}{2} \left| \int_{-\infty}^{\infty} dz \phi^*_{n,k_t=0}(z) M_b g_m^{(3)}(k_t, z) \right|^2 \\ M_b^2 = \frac{|\langle S|p_x|X \rangle|^2}{3} = \frac{m_0}{6} E_p. \quad (\text{A.70})$$

where M_b^2 is the bulk momentum matrix element squared and E_p is the corresponding energy parameter. $g_m^{(1)}(k_t, z)$ and $g_m^{(2)}(k_t, z)$ are the eigencomponents of the upper Hamiltonian H_U ; $g_m^{(3)}(k_t, z)$ and $g_m^{(4)}(k_t, z)$ are the eigencomponents of the lower Hamiltonian H_L , and ϕ is the eigenfunction for the Γ valley. Similar equations may be obtained for TM waves [13].

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