Optical transitions in semiconductor superlattices with zinc-blende structure in the $\mathbf{k}\cdot\mathbf{p}$ approximation

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Transition-matrix elements for superlattices consisting of materials with the zinc-blende structure are presented in analytical form in the $\mathbf{k}\cdot\mathbf{p}$ approximation including the Γ_6, Γ_7, and Γ_8 bands. The resulting selection rules for cases where the magnetic field is absent, and where the magnetic field is applied perpendicular to the superlattice layers, are discussed. The results can be used for type-I, -II, and -III superlattices. They can also be used for other systems, such as a single quantum well.

I. INTRODUCTION

Semiconductor superlattices comprised of alternating layers of two semiconductor materials having the zinc-blende structure are of major scientific and technological importance. Both optical and magneto-optical studies of such superlattices provide powerful tools for investigating band parameters of these multilayer systems. For magneto-optical transitions, the simplest situation for which the band structure can be calculated corresponds to the geometry where the magnetic field is applied perpendicular to the superlattice layers, and the band structure for this geometry has been studied theoretically using various $\mathbf{k}\cdot\mathbf{p}$ models[1-9] involving both conduction and valence bands. However, the selection rules for transitions between Landau levels in different configurations have so far been limited only to numerical calculations. In this paper we will present, *analytically*, the transition-matrix elements as well as the corresponding selection rules.

In a superlattice, each bulk band is quantized into subbands. Depending on the bulk bands to which the subbands belong, labels E, lh, and hh are often used to represent the electron, light-hole, and heavy-hole subbands, respectively. The quantum number of the subband N is often added to the labels after the letters (e.g., $E1$ and hh2). If a magnetic field is applied, each subband will again be quantized into Landau levels with quantum number n.

The purpose of this paper is to find the symmetry properties of the wave functions of the subbands, or Landau levels in the presence of a magnetic field (instead of their exact forms, which are usually complicated) and—using these symmetry properties—to formulate the transition-matrix elements in analytical form. The procedure is, then, to first find the symmetry properties of the wave functions, in the general case when a magnetic field is present, and to obtain the transition-matrix elements with wave functions in the $\mathbf{k}\cdot\mathbf{p}$ approximation. The resulting selection rules for transitions between Landau levels will then be discussed. The results presented in this paper can be used for both intersubband and intrasubband transitions in type-I, -II, and -III superlattices, as long as the constituent materials have direct energy gaps. They can also be applied to some other cases (e.g., a single square quantum well) which will be discussed at the end of the paper.

We will then discuss the special case of vanishing magnetic field, describing the limitations of the well-known selection rule $\Delta N=0$ used for interband transitions.[10] Transitions induced by higher-order perturbations (such as the effects of inversion asymmetry and warping) will not be discussed here, although such effects can in principle be included in the form of perturbations when this becomes necessary.

We assume that the $\mathbf{k}\cdot\mathbf{p}$ approximation can be applied to both constituent materials near the Γ point, and to the superlattice as well. In Sec. II, we will first briefly review the forms of the wave equations and of the wave functions for the bulk case. We will then discuss the symmetries of the wave functions in a superlattice in the general form, with an external magnetic field present. Taking the wave-function symmetries into account, we will find the transition-matrix elements and the selection rules for magneto-optical transitions, which will be presented in Sec. III. In Sec. IV we discuss the special case of $\mathbf{B}=\mathbf{0}$. Finally, we will discuss the applicability of the results presented in the paper.

II. SYMMETRIES OF SUPERLATTICE WAVE FUNCTIONS

For convenience in later discussions, we will briefly review the theory of the band structure of bulk crystals with a zinc-blende structure. Zinc-blende-structure materials have been thoroughly studied,[11,12] and it is well known that the bands of importance to optical properties are the s-like Γ_6 band, and the p-like Γ_7 and Γ_8 bands, each of which has a double degeneracy at the Γ point related to the spin-up and spin-down states. Different sets of basis functions with Γ_6, Γ_7, and Γ_8 symmetries have been used by various authors for studies involving band structures,[13,14] but the differences between the various formalisms usually consist only of factors of $\pm i$ or -1 for some of the components of the basis. We will use the basis employed in Ref. 14, in the following order, for the eight $u_i(\mathbf{r})$ components:

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$$
\begin{aligned}
u_1(\mathbf{r}) &= |S\uparrow\rangle \ , \\
u_3(\mathbf{r}) &= \left|\frac{-i}{\sqrt{2}}(X+iY)\uparrow\right\rangle \ , \\
u_5(\mathbf{r}) &= \left|\frac{i}{\sqrt{6}}[(X-iY)\uparrow+2Z\downarrow]\right\rangle \ , \\
u_7(\mathbf{r}) &= \left|\frac{-i}{\sqrt{3}}[(X-iY)\uparrow-Z\downarrow]\right\rangle \ , \\
u_2(\mathbf{r}) &= |S\downarrow\rangle \ , \\
u_4(\mathbf{r}) &= \left|\frac{i}{\sqrt{2}}(X-iY)\downarrow\right\rangle \ , \\
u_6(\mathbf{r}) &= \left|\frac{-i}{\sqrt{6}}[(X+iY)\downarrow-2Z\uparrow]\right\rangle \ , \\
u_8(\mathbf{r}) &= \left|\frac{-i}{\sqrt{3}}[(X+iY)\downarrow+Z\uparrow]\right\rangle \ ,
\end{aligned}
\tag{1}
$$

where S is a function which transforms as a scalar; X, Y, and Z are functions with the symmetries of the coordinates x, y, and z, respectively; and the symbols $\uparrow$ and $\downarrow$ represent spin-up and spin-down states, respectively.

The wave function for a band labeled by μ, with a wave vector $\mathbf{k}$, can then be written as[12]

$$
\Phi_{\mu,k}(\mathbf{r}) = \sum_{i=1}^{8} u_i(\mathbf{r}) f_{\mu,i,k}(\mathbf{r}) \ , \tag{2}
$$

where i runs over the doubly degenerate Γ_6 band, the two Γ_8 bands and the Γ_7 band. Also, in the above equation $u_i(\mathbf{r})$ is the Bloch function of the ith band at the Γ point, and $f_{\mu,i,k}(\mathbf{r})$ are the envelope functions. It has been shown[12] that the Schrödinger equation of this system can be written as a set of coupled differential equations in the following form:

$$
\sum_{i=1}^{8} H_{ji} f_i(\mathbf{r}) = E f_j(\mathbf{r}) \ ,
$$

where the subscripts μ and k have been omitted. The interactions between the Γ_6, the Γ_7, and the Γ_8 bands are treated exactly, while the effects of higher bands are handled by perturbation theory up to terms in k^2. The effects of inversion asymmetry and warping are neglected in the following discussions. Using a certain basis, $u_i(\mathbf{r})$, H_{ji} can be collectively represented in the matrix form by an 8×8 matrix,[13]

$$
\underline{H}^B = \begin{bmatrix} \underline{H}_a & \underline{H}_c \\ \underline{H}_c^{\dagger} & \underline{H}_b \end{bmatrix} \ , \tag{3}
$$

where $\underline{H}_a$, $\underline{H}_b$, and $\underline{H}_c$ are all 4×4 matrices, $\underline{H}_c$ being proportional to k_z, while $\underline{H}_a$ and $\underline{H}_b$ contain terms of zeroth order and second order in k_z. At $k_z=0$, $\underline{H}_c=\underline{0}_{4\times 4}$, and $\underline{H}^B$ is then decoupled into $\underline{H}_a$ and $\underline{H}_b$. The superscript B on the matrix $\underline{H}^B$ stands for bulk. The results obtained, respectively, from $\underline{H}_a$ and $\underline{H}_b$ are often called the a-set and the b-set solutions.

The superlattice system which we wish to discuss is of the most common form, made up of alternating layers of materials I and II, both with zinc-blende lattices, as shown in Fig. 1, where d_1 and d_2 are the thicknesses of materials I and II, respectively. The magnetic field is in the z direction, the growth direction of the superlattice. With the origin of the z axis chosen at the center of a layer consisting of material I, the Hamiltonian matrix can be written as

$$
\underline{H}^S = \begin{cases} \underline{H}_{\mathrm{I}}^B, & md - d_1/2 < z < md + d_1/2 \\ \underline{H}_{\mathrm{II}}^B, & md + d_1/2 < z < md + d_1/2 + d_2 \end{cases} \qquad m = 0, \pm 1, \pm 2, \ldots \tag{4}
$$

where $d=d_1+d_2$, and $\underline{H}_{\mathrm{I}}^B$ and $\underline{H}_{\mathrm{II}}^B$ are the matrices $\underline{H}^B$ corresponding to *bulk* materials I and II, respectively. The superscript S stands for superlattice. Since k_z is generally nonzero and does not commute with the superlattice Hamiltonian, we replace it by $-i(\partial/\partial z)$. Unlike the bulk case, now the decoupling of $\underline{H}_a$ and $\underline{H}_b$ at $k_z=0$ can no longer be achieved.

In our analysis we will make the assumption that the basis sets $u_i(\mathbf{r})$ in the two materials are the same. The validity of this assumption has been justified for many cases, such as for HgTe/CdTe and GaAs/$Ga_{1-x}Al_xAs$ superlattices.[9] The wave functions of the superlattice can then be simply expressed as

$$
\Phi(\mathbf{r}) = \sum_{i=1}^{8} u_i(\mathbf{r}) f_i(\mathbf{r}) \ . \tag{5}
$$

Here $f_i(\mathbf{r})$ are the envelope functions in the superlattice, satisfying

$$
\underline{H}^S \underline{F}(r) = E \underline{F}(\mathbf{r}) \ , \tag{6}
$$

where $\underline{F}(\mathbf{r})$ is the matrix form of $f_i(\mathbf{r})$. Looking at Eqs. (6) and (4), we see that $\underline{F}(\mathbf{r})$ has to satisfy $\underline{H}_{\mathrm{I}}^B$ and $\underline{H}_{\mathrm{II}}^B$ individually in corresponding materials. Furthermore, $\underline{F}(\mathbf{r})$ is required to meet the conditions set by the symmetry and the periodicity of the superlattice, and the conditions of continuity[1,3] at the interfaces. We write $\underline{F}(\mathbf{r})$ as

$$
\underline{F}(\mathbf{r}) = \begin{bmatrix} \underline{f}_a(\mathbf{r}) \\ \underline{f}_b(\mathbf{r}) \end{bmatrix} \ , \tag{7}
$$

where $\underline{f}_a(\mathbf{r})$ and $\underline{f}_b(\mathbf{r})$ are the components correspond-

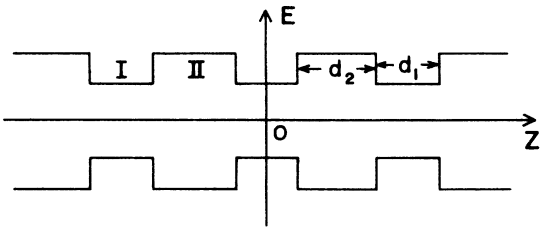

FIG. 1. Schematic representation of a superlattice used to illustrate the structure of a superlattice and to define parameters.

ing to the a-set and the b-set basis, respectively, with[12]

$$\underline{f}_a(\mathbf{r})=\begin{bmatrix} f_1(\mathbf{r}) \\ f_3(\mathbf{r}) \\ f_5(\mathbf{r}) \\ f_7(\mathbf{r}) \end{bmatrix} \quad \text{and} \quad \underline{f}_b(\mathbf{r})=\begin{bmatrix} f_2(\mathbf{r}) \\ f_4(\mathbf{r}) \\ f_6(\mathbf{r}) \\ f_8(\mathbf{r}) \end{bmatrix} .$$

Since, as has been pointed out, $\underline{H}^S$ can no longer be decoupled into $\underline{H}_a$ and $\underline{H}_b$ in a superlattice, both $\underline{f}_a(\mathbf{r})$ and $\underline{f}_b(\mathbf{r})$ are in general nonzero for a given superlattice state.

As stated at the beginning, our task is to find the transition-matrix elements. As will be seen, this can be accomplished by considering symmetries of wave functions of initial and final states. We will thus avoid the calculations of the band structure and the wave functions, and will concentrate on the symmetry properties of the wave functions in general.

It is well known that, even for the one-band case of a superlattice (the Kronig-Penney model), the solutions of the eigenvalues and eigenfunctions can be quite complicated.[15] However, the symmetries are rather simple. The same is true for our case, where several bands (i.e., Γ_6, Γ_7, and Γ_8 bands) and the spin are considered. Therefore, the constraint applied on the wave equation by the symmetry of the superlattice should automatically give us the symmetries of the eigenstates.

With the magnetic field applied in the z direction, the motion in the x-y plane (the in-plane motion for the superlattice) will be quantized into Landau levels. Thus we can write $f_i(\mathbf{r})$, the components of $F(\mathbf{r})$, in the following form:

$$f_i(\mathbf{r})=\phi_{n(i)}(x,y)\psi_i(z) , \tag{8}$$

where $\phi_{n(i)}(x,y)$ is the wave function in the x-y plane in the form of the $n(i)$th Landau level of a free electron, and $\psi_i(z)$ is the envelope function in the z direction.

Since in the present model inversion asymmetry is not considered, the superlattice is symmetric with a reflection through $z=0$, denoted by an operator R. Therefore the wave equation should be invariant under such a reflection. Inspecting Eqs. (3) and (4), we find that $\underline{H}^S$ itself is not invariant in form under the reflection R, because $\underline{H}_c$ is proportional to $\partial/\partial z$. However, the difference between $R\underline{H}^S$ and $\underline{H}^S$ is only that given by a unitary transformation. That is

$$R\underline{H}^S=\underline{U}^{-1}\underline{H}^S\underline{U} , \tag{9}$$

with $\underline{U}$ being either

$$\underline{U}=\begin{bmatrix} \underline{I}_4 & \underline{0}_{4\times4} \\ \underline{0}_{4\times4} & -\underline{I}_4 \end{bmatrix} , \tag{10}$$

or

$$\underline{U}=\begin{bmatrix} -\underline{I}_4 & \underline{0}_{4\times4} \\ \underline{0}_{4\times4} & \underline{I}_4 \end{bmatrix} , \tag{11}$$

where $\underline{I}_4$ is the 4×4 unit matrix. Since $\underline{H}^S$ is not formally invariant under the operation R, the envelope function $\underline{F}(\mathbf{r})$ is not an eigenfunction of R. The invariance can be stated as follows: if Eq. (6) gives the wave function $\underline{F}(\mathbf{r})$ and the energy E of a state, so does the equation

$$R[\underline{H}^S\underline{F}(\mathbf{r})]=R[E\underline{F}(\mathbf{r})] . \tag{12}$$

With Eq. (9), the above equation yields

$$\underline{H}^S\{\underline{U}[R\underline{F}(\mathbf{r})]\}=E\{\underline{U}[R\underline{F}(\mathbf{r})]\} . \tag{13}$$

Comparing this equation with Eq. (6), one finds that if the state is not degenerate,

$$\underline{F}(\mathbf{r})=\underline{U}[R\underline{F}(\mathbf{r})] , \tag{14}$$

with a properly chosen phase factor. [If the state *is* degenerate, one can always find linear combinations of $\underline{F}(\mathbf{r})$'s of the degenerate states such that Eq. (14) is satisfied.]

Taking $\underline{U}$ given by Eq. (10), we get

$$\begin{bmatrix} \underline{f}_a(\mathbf{r}) \\ \underline{f}_b(\mathbf{r}) \end{bmatrix}=\begin{bmatrix} R\underline{f}_a(\mathbf{r}) \\ -R\underline{f}_b(\mathbf{r}) \end{bmatrix} .$$

Thus, in the above $\underline{f}_a(\mathbf{r})$ is an even function of z, denoted by $\underline{f}^e_a(\mathbf{r})$, while $\underline{f}_b(\mathbf{r})$ is an odd function of z, denoted by $\underline{f}^o_b(\mathbf{r})$. If, on the other hand, one uses $\underline{U}$ given by Eq. (11), one will have

$$\begin{bmatrix} \underline{f}_a(\mathbf{r}) \\ \underline{f}_b(\mathbf{r}) \end{bmatrix}=\begin{bmatrix} -R\underline{f}_a(\mathbf{r}) \\ R\underline{f}_b(\mathbf{r}) \end{bmatrix} .$$

Thus now $\underline{f}_a(\mathbf{r})$ is an odd function of z, labeled $\underline{f}^o_a(\mathbf{r})$, and $\underline{f}_b(\mathbf{r})$ is an even function of z, labeled $\underline{f}^e_b(\mathbf{r})$.

As a result of the invariance discussed above, we find that there can only be *two* kinds of eigenfunctions for the superlattice Hamiltonian (and their linear combinations, if they are degenerate), having the forms

$$\underline{F}_A(\mathbf{r})=\begin{bmatrix} \underline{f}^e_a(\mathbf{r}) \\ \underline{f}^o_b(\mathbf{r}) \end{bmatrix}, \quad \underline{F}_B(\mathbf{r})=\begin{bmatrix} \underline{f}^o_a(\mathbf{r}) \\ \underline{f}^e_b(\mathbf{r}) \end{bmatrix} , \tag{15}$$

where we have assigned the subscripts A and B to $\underline{F}(\mathbf{r})$ with $\underline{f}^e_a(\mathbf{r})$ and $\underline{f}^e_b(\mathbf{r})$, respectively. States having $\underline{F}_A(\mathbf{r})$ and $\underline{F}_B(\mathbf{r})$ will be referred to as A-set and B-set states, respectively, for convenience. (Capital letter subscripts A and B are used for superlattice states, which are to be distinguished from bulk cases.) In a magnetic field, the states are generally nondegenerate. As we will be shown later, states are doubly degenerate if $B=0$, in which case we will still keep the wave functions given in Eq. (15) as the eigenfunctions of the superlattice Hamiltonian. One may have noticed that $\underline{F}_A(\mathbf{r})$ and $\underline{F}_b(\mathbf{r})$ are not eigenfunctions of the operator R, which is the direct result of the lack of formal invariance of $\underline{H}^S$ under the operation R.

It should be emphasized that the superlattice states with wave functions $\underline{F}_A(\mathbf{r})$ and $\underline{F}_B(\mathbf{r})$ defined above by their symmetries do not always correspond, respectively, to the a-set and b-set bulk states for all the subbands. This is because the subbands of a superlattice originating from the same bulk band may have different symmetries, which is most obvious in the one-band case where wave functions of the subbands originating from the only band have different symmetries.

III. SELECTION RULES

We are now ready to formulate the transition-matrix elements. To do so, we will express the wave functions $\underline{F}_A(\mathbf{r})$ and $\underline{F}_B(\mathbf{r})$, with components in the form shown in Eq. (8). With the basis given in Eq. (1), the components $f_i(\mathbf{r})$ of the two kinds of envelope functions for the superlattice can be written in matrix form as[13,14]

$$\underline{F}^n_A(\mathbf{r})=\begin{bmatrix}\phi_n\psi^e_{1,n}(z)\\ \phi_{n-1}\psi^e_{3,n}(z)\\ \phi_{n+1}\psi^e_{5,n}(z)\\ \phi_{n+1}\psi^e_{7,n}(z)\\ \phi_{n+1}\psi^o_{2,n}(z)\\ \phi_{n+2}\psi^o_{4,n}(z)\\ \phi_n\psi^o_{6,n}(z)\\ \phi_n\psi^o_{8,n}(z)\end{bmatrix},$$

$$\underline{F}^n_B(\mathbf{r})=\begin{bmatrix}\phi_n\psi^o_{1,n}(z)\\ \phi_{n-1}\psi^o_{3,n}(z)\\ \phi_{n+1}\psi^o_{5,n}(z)\\ \phi_{n+1}\psi^o_{7,n}(z)\\ \phi_{n+1}\psi^e_{2,n}(z)\\ \phi_{n+2}\psi^e_{4,n}(z)\\ \phi_n\psi^e_{6,n}(z)\\ \phi_n\psi^e_{8,n}(z)\end{bmatrix}, \tag{16}$$

where again the superscripts e and o represent even and odd parities, respectively, and n is the Landau-level quantum number. Again, we use capital letters A and B to differentiate the superlattice case from the bulk. Here n indicates the quantum number of the Landau levels in the band structure, whose wave function $\underline{F}^n_A(\mathbf{r})$ or $\underline{F}^n_B(\mathbf{r})$ consists of components $\phi_{n(i)}\psi_{i,n}(z)$, $n(i)$ being the quantum number for $\phi_{n(i)}$. The two functions in Eq. (16) differ, in form, only by an interchange of the superscripts e and o.

The wave functions given in Eq. (16) are different from their bulk counterparts in several ways. First of all, the parts of the wave functions in the z direction are no longer plane wave functions, as is the case in the bulk. Instead, they are functions of z with particular parities. Since k_z is generally not zero in a superlattice, all eight components of the wave functions are, in principle, nonvanishing. In the bulk case, however, based on density-of-states considerations, k_z can be assumed to be zero for most situations of interest, which leads to the decoupling of $\underline{H}_a$ and $\underline{H}_b$, leaving only four nonvanishing components [either the top four, or the bottom four components of the eight-component wave functions given in Eq. (16)]. The mixing of the a-set and b-set bulk states in a superlattice depends on the energy gaps of the bulk materials. A smaller energy gap gives stronger mixing.

With the symmetries of the superlattice wave functions known, we can find the matrix elements for transitions both within each set [e.g., within $\underline{F}^n_A(\mathbf{r})$], and between the two sets [i.e., between $\underline{F}^n_A(\mathbf{r})$ and $\underline{F}^n_B(\mathbf{r})$]. In the $\mathbf{k}\cdot\mathbf{p}$ approximation, the Hamiltonian of the interaction between an electron and the electromagnetic wave is[16]

$$H'=\frac{eE}{2m\omega}\left[\mathbf{p}+\frac{e\,\mathbf{A}}{c}\right]\cdot\hat{\boldsymbol{\varepsilon}},$$

without the phase factor of the electromagnetic wave, where E, $\mathbf{A}$, and ω are the electric field, the vector potential, and the angular frequency of the electromagnetic wave, respectively; m is the free-electron mass; and the polarization of the wave is represented by $\hat{\boldsymbol{\varepsilon}}$. The transition-matrix elements between an initial state Φ_I and a final state Φ_F [both having the form shown in Eq. (2)] can be written as

$$\langle\Phi_F|H'|\Phi_I\rangle=\sum_{i,i'}[\langle u_{i'}(\mathbf{r})|u_i(\mathbf{r})\rangle\langle f_{i'}(\mathbf{r})|H'|f_i(\mathbf{r})\rangle + \langle u_{i'}(\mathbf{r})|H'|u_i(\mathbf{r})\rangle\langle f_{i'}(\mathbf{r})|f_i(\mathbf{r})\rangle], \tag{17}$$

because $u_i(\mathbf{r})$'s are the Γ-point Bloch functions varying with periods of the size of a unit cell of the bulk crystals, while the envelope functions $f_i(\mathbf{r})$ are slow varying.

The first and second terms in Eq. (17) are often referred to as the intraband and the interband term, respectively. However, in most II-VI and III-V compound semiconductors (e.g., in superlattices involving GaAs, CdTe, or HgTe), the second term in Eq. (17) is much greater than the first for both intraband and interband transitions because of the large values of the momentum matrix element $P\equiv-(i\hbar/m)\langle S|P_x|X\rangle$ characteristic of these materials. Only when the band gap is very large (e.g., for systems involving ZnSe) will the first term be of significance for intraband transitions. Therefore in what follows we will first discuss the second term. We then obtain the matrix elements for transitions within the A set:

$$\langle\Phi_A(n')|H'|\Phi_A(n)\rangle=\frac{eEP}{2\sqrt{3}\hbar\omega}\{[(\sqrt{3}Z^e_{3,1,n',n}-Z^e_{1,5,n',n}+\sqrt{2}Z^e_{1,7,n',n}) + (Z^o_{6,2,n',n}+\sqrt{2}Z^o_{8,2,n',n}-\sqrt{3}Z^o_{2,4,n',n})]\varepsilon_-\delta_{n',n+1}+[n'\rightleftharpoons n]\varepsilon_+\delta_{n',n-1}\}. \tag{18a}$$

Similarly, matrix elements for transitions within the set B are

$$\langle\Phi_B(n')|H'|\Phi_B(n)\rangle=\frac{eEP}{2\sqrt{3}\hbar\omega}\{[(\sqrt{3}Z^o_{3,1,n',n}-Z^o_{1,5,n',n}+\sqrt{2}Z^o_{1,7,n',n}) + (Z^e_{6,2,n',n}+\sqrt{2}Z^e_{8,2,n',n}-\sqrt{3}Z^e_{2,4,n',n})]\varepsilon_-\delta_{n',n+1}+[n'\rightleftharpoons n]\varepsilon_+\delta_{n',n-1}\}, \tag{18b}$$

and for transitions between sets A and B, we have

$$\langle \Phi_B(n')|H'|\Phi_A(n)\rangle = -\frac{eEP}{\sqrt{3}\hbar\omega}[(\sqrt{2}Z^e_{2,5,n',n}+Z^e_{2,7,n',n}+\sqrt{2}Z^e_{6,1,n',n}-Z^e_{8,1,n',n}) + (\sqrt{2}Z^o_{5,2,n',n}+Z^o_{7,2,n',n}+\sqrt{2}Z^o_{1,6,n',n}-Z^o_{1,8,n',n})]\varepsilon_z\delta_{n',n} \ . \quad (18c)$$

Here $Z^{\nu}_{i',i,n',n}$ (with ν being either e or o) is defined by

$$Z^{\nu}_{i',i,n',n} = \langle \psi^{\nu}_{i',n'}(z)|\psi^{\nu}_{i,n}(z)\rangle \ , \quad (19)$$

and $[n' \Longleftrightarrow n]$ denotes a term which is the same as the preceding term, but with n' and n interchanged. For the polarizations, we have used

$$\varepsilon_+ = \frac{1}{\sqrt{2}}(\varepsilon_x + i\varepsilon_y), \quad \varepsilon_- = \frac{1}{\sqrt{2}}(\varepsilon_x - i\varepsilon_y) \ ,$$

which represent the polarizations of CRI (cyclotron-resonance-inactive, or σ_R) and CRA (cyclotron-resonance-active, or σ_L) polarizations, respectively. In Eq. (18c), ε_z corresponds to the $\mathbf{E}\|\mathbf{B}$, or π, polarization.

Equations (18a) and (18b) describe transitions elicited by the circularly polarized electromagnetic waves having $\mathbf{q}\|\mathbf{B}$, where $\mathbf{q}$ is the wave vector of the radiation. Equation (18c) requires a linearly polarized electromagnetic wave having $\hat{\boldsymbol{\varepsilon}}\|\mathbf{B}$, which implies $\mathbf{B}\perp\mathbf{q}$. In order to keep $\mathbf{B}$ in the z direction—i.e., along the axis of the superlattice—$\mathbf{q}$ must then be in the plane of the layers. In practice, experiments involving the ε_z polarization can be carried out in the so-called strip-line technique.[17]

Now we will present the selection rules implied by Eq. (18), according to the familiar bulk a-set and b-set states. To do this, we first discuss the relation between the states represented by $\underline{F}_A(\mathbf{r})$ and $\underline{F}_B(\mathbf{r})$ and the corresponding bulk states. In the one-band case, different subbands in a superlattice are characterized by the different parities and the number of extrema of the wave functions in the superlattice unit cell. If the lowest subband is designated with $N=1$, all the subbands with $N=2m-1$ ($m=1,2,3,\ldots$) have functions of z even under the reflection operation R. Meanwhile, all the subbands with $N=2m$ have odd functions of z. Also, the number of extrema of the Nth subband is equal to N in a well of the superlattice.[10] In our case (where several bands and the spin are considered), the situation is analogous in that the different subbands originating from one particular band (with relatively weaker mixing from the other bands) are distinguished by wave functions with different symmetries (and the number of extrema within the superlattice unit cell).

With wave functions given in Eq. (16) and the basis given in Eq. (1), one finds that all the Landau levels in the spin-up $E1$ subband [with $f_1(\mathbf{r})$ being the major component of the wave function originating from the a set in the bulk] have wave functions in the form of $\underline{F}^n_A(\mathbf{r})$ in Eq. (16), because they have $f_1(\mathbf{r})$ even in z, as a result of $N=1$. The Landau levels in the spin-up $E2$ subband [again with $f_1(\mathbf{r})$ being the major component] have wave functions described by $\underline{F}^n_B(\mathbf{r})$, because $N=2$. In the same way, one finds that the Landau levels in the spin-down $E1$ and $E2$ subbands [both having $f_2(r)$ as major components, originating from the bulk b set] have wave functions $\underline{F}^n_B(\mathbf{r})$ and $\underline{F}^n_A(\mathbf{r})$, respectively. In general, if $N=2m-1$, $\underline{F}^n_A(\mathbf{r})$ and $\underline{F}^n_B(\mathbf{r})$ correspond to the bulk a-set and b-set states, respectively. When $N=2m$, $\underline{F}^n_A(\mathbf{r})$ and $\underline{F}^n_B(\mathbf{r})$, respectively, originate from the bulk b-set and a-set states.

It has been pointed out that only subbands with the same quantum number N have significant overlap in their wave functions.[18] This, however, is only true when the interactions between different bands can be neglected. From the symmetries of the wave functions in the one-band case (either even or odd in z, depending on the quantum number N), the coexistence of components both even and odd in z in the wave function given in Eq. (16) can be understood as the result of the mixing of subbands belonging to the bulk a set and b set with different symmetries (having different quantum numbers N). Such a mixing cannot be solved exactly even in the simple case of two bands coupled through $\partial/\partial z$, with barrier heights being infinite in both bands. In this simple case, however, we find that if the coupled component is taken to be a linear combination of the wave functions of all the subbands without coupling (i.e., the wave functions of subbands in a one-band single quantum well with infinite barriers, which can be solved exactly) satisfying the symmetry requirement discussed before, the dominant contributions are from the subbands with quantum numbers $N\pm1$. This indicates that the wave functions given in Eq. (16) will lead to a substantial overlap between the wave functions of subbands with $\Delta N=\pm1$, if the k_z coupling is strong.

With the above discussions the selection rules for specific polarizations can be obtained from Eq. (18) by identifying terms associated with ε_+, ε_-, and ε_z, as follows:

$$\begin{aligned} &\text{CRA (or } \sigma_L\text{)}: \ a_n \rightarrow a_{n+1}, \ b_n \rightarrow b_{n+1} \ , \\ &\text{CRI (or } \sigma_R\text{)}: \ a_n \rightarrow a_{n-1}, \ b_n \rightarrow b_{n-1} \ , \\ &\mathbf{E}\|\mathbf{B} \text{ (or } \pi\text{)}: \ a_n \leftrightarrow b_n \ , \end{aligned} \quad (20a)$$

for $\Delta N=0$, and

$$\begin{aligned} &\text{CRA}: \ a_n \rightarrow b_{n+1}, \ b_n \rightarrow a_{n+1} \ , \\ &\text{CRI}: \ a_n \rightarrow b_{n-1}, \ b_n \rightarrow a_{n-1} \ , \\ &\mathbf{E}\|\mathbf{B}: \ a_n \leftrightarrow a_n, \ b_n \leftrightarrow b_n \ , \end{aligned} \quad (20b)$$

for $\Delta N=\pm1$, which is induced by the k_z coupling between the a set and the b set.

Comparing Eq. (20a) with the selection rules for bulk crystals,[14] we see that in the CRA and CRI configurations, the selection rules for both cases are the same. In the $\mathbf{E}\|\mathbf{B}$ configuration (with $\mathbf{B}$ perpendicular to the layers in the superlattice), the selection rules appear

to be different from the bulk case, because in Eq. (20a) $\Delta n=0$ for all the allowed transitions. This is caused simply by the fact that in a superlattice the coupling of H_a and H_b makes the assignments of $n(i)$ to the components belonging to H_a and H_b different from that used in Ref. 14, where the assignments of n to H_a and to H_b are independent. In fact, the transitions allowed in $\mathbf{E}\|\mathbf{B}$ given above, which look like spin-flip transitions, correspond to the so-called combined resonance in the bulk case. Therefore the selection rules for intrasubband transitions and interband transitions with $\Delta N=0$ are the same as in the bulk case.

The intersubband transitions given in Eq. (20b), having no counterpart in the bulk case, are induced by the coupling through k_z. The intensity of such transitions will therefore depend on the coupling. They will be stronger for superlattices with smaller energy gaps, such as HgTe-CdTe superlattices. As we can see in Eq. (20b), transitions within the same set (either the a set or the b set) occur in the configuration with $\mathbf{E}\|\mathbf{B}$. In contrast to bulk magnetoptics, transitions between the a set and the b set can only be seen in the CRA and CRI configurations.

So far we have focused on the transitions allowed by the second term in Eq. (17). As mentioned earlier, the first term in Eq. (17) cannot be neglected for intraband transitions when the band gap is very large. The reason for this is that for large band gaps the mixing of the conduction band and the valence bands is small, resulting in small values of the intraband transition-matrix elements from the second term in Eq. (17). To obtain the transition-matrix elements resulting from the first term, it is easier to introduce the "raising" and "lowering" operators, defined as

$$a^{\dagger}=\frac{1}{\hbar\sqrt{2s}}(P_x+iP_y)\ ,$$

$$a=\frac{1}{\hbar\sqrt{2s}}(P_x-iP_y)\ ,$$

respectively, where

$$s=\frac{eB}{\hbar c}$$

and

$$\mathbf{P}=\mathbf{p}+\frac{e\,\mathbf{A}}{c}\ .$$

Then H' becomes

$$H'=\frac{eE}{2m\omega}[\hbar\sqrt{s}\,(a^{\dagger}\varepsilon_-+a\varepsilon_+)+P_z\varepsilon_z]\ . \tag{21}$$

For simplicity of discussion in this case, we replace the superscripts "e" and "o" representing the parities by the subband quantum number N. The transition-matrix elements can now be written as

$$\langle\Phi_{N'}(n')|H'|\Phi_N(n)\rangle=\frac{eE\hbar}{2m\omega}\left[\left[\sum_i\sqrt{[n(i)+1)]s}\,\langle\psi^{N'}_{i,n'}(z)|\psi^{N}_{i,n}(z)\rangle\right]\delta_{n',\,n+1}\varepsilon_-+\left[\sum_i\sqrt{n(i)s}\,\langle\psi^{N'}_{i,n'}(z)|\psi^{N}_{i,n}(z)\rangle\right]\delta_{n',\,n-1}\varepsilon_+\right.$$
$$\left.-i\left[\sum_i\left\langle\psi^{N'}_{i,n'}(z)\left|\frac{\partial}{\partial z}\right|\psi^{N}_{i,n}(z)\right\rangle\right]\delta_{n',n}\varepsilon_z\right]\ , \tag{22}$$

where $\Phi_{N'}(n')$ is from either the A set or the B set, and so is $\Phi_N(n)$.

With the symmetries of the wave functions discussed earlier, the resulting selection rules are found to be exactly the same, in form, as that in Eqs. (20a) and (20b). However, since the transition-matrix elements given in Eq. (22) are only significant in wide-gap superlattices, we should exclude the transitions resulting from the mixing of the conduction band and the valence bands. Thus the dominant intraband transitions follow the selection rules

$$\begin{aligned}&\text{CRA: } a_n\to a_{n+1},\ \ b_n\to b_{n+1}\ ,\\ &\text{CRI: } a_n\to a_{n-1},\ \ b_n\to b_{n-1}\ ,\end{aligned} \tag{23a}$$

for $\Delta N=0$, and

$$\mathbf{E}\|\mathbf{B}\text{: } a_n\to a_n,\ \ b_n\to b_n \tag{23b}$$

for $\Delta N=\pm1$. The interband transitions in this case will still follow the selection rules resulting from the second term (i.e., the interband term), namely, Eqs. (20a) and (20b). But the transitions described in Eq. (20b) become negligible because of the weak mixing of the conduction band and the valence bands.

IV. THE CASE OF B=0

In this section we will first discuss the degeneracy of the eigenstates arising when the magnetic field is zero. We will then write the transition-matrix elements for this special case, and we will discuss the corresponding transitions.

When $\mathbf{B}=0$, we have[13] $\underline{H}_a=\underline{H}_b$, in addition to $\underline{H}_c^{\dagger}=\underline{H}_c$. Under this condition

$$\underline{H}^S=\underline{U}^{-1}\underline{H}^S\underline{U}\ , \tag{24}$$

where

$$\underline{U}=\begin{bmatrix}\underline{0}_{4\times4} & \underline{I}_4\\ \underline{I}_4 & \underline{0}_{4\times4}\end{bmatrix}\ , \tag{25}$$

with $\underline{I}_4$ being the 4×4 unit matrix. We assume that a wave function

$$\underline{F}(\mathbf{r})=\begin{bmatrix}\underline{f}^{e}(\mathbf{r})\\ \underline{f}^{o}(\mathbf{r})\end{bmatrix}, \tag{26}$$

given in Eq. (15) as $\underline{F}_{A}(\mathbf{r})$, is an eigenfunction of Eq. (6). (The subscripts a and b have now been omitted.) Replacing $\underline{H}^{S}$ in Eq. (6) by $\underline{U}^{-1}\underline{H}^{S}\underline{U}$ according to Eq. (24), and multiplying by $\underline{U}$ from the left, we obtain

$$\underline{H}^{S}\underline{U}\,\underline{F}(\mathbf{r})=E\underline{U}\,\underline{F}(\mathbf{r}) .$$

This means that $\underline{U}\,\underline{F}(\mathbf{r})$ is also an eigenfunction with the same energy E. Explicitly,

$$\underline{U}\,\underline{F}(\mathbf{r})=\begin{bmatrix}\underline{f}^{o}(\mathbf{r})\\ \underline{f}^{e}(\mathbf{r})\end{bmatrix} .$$

One finds that $\underline{U}\,\underline{F}(\mathbf{r})$ given above has the form of $\underline{F}_{B}(\mathbf{r})$ given in Eq. (15). Thus, every eigenstate of $\underline{H}^{S}$ with an A-set wave function is degenerate with a B-set eigenstate at $\mathbf{B}=\mathbf{0}$. In the same way we can prove that every B-set eigenstate is degenerate with an A-set eigenstate at $\mathbf{B}=\mathbf{0}$. Such a degeneracy is the direct result of the degenerate spin states in bulk materials without external magnetic fields.

When $\mathbf{B}=\mathbf{0}$, both k_x and k_y commute with H^{S}, as in the bulk case.[14] Thus we can replace the Landau level wave functions in Eq. (16) with plane wave functions for the in-plane motion, which gives

$$\underline{F}_{A}(\mathbf{r})=e^{ik_x x}e^{ik_y y}\begin{bmatrix}\psi_1^{e}(z)\\ \psi_3^{e}(z)\\ \psi_5^{e}(z)\\ \psi_7^{e}(z)\\ \psi_2^{o}(z)\\ \psi_4^{o}(z)\\ \psi_6^{o}(z)\\ \psi_8^{o}(z)\end{bmatrix},$$

$$\underline{F}_{B}(\mathbf{r})=e^{ik_x x}e^{ik_y y}\begin{bmatrix}\psi_1^{o}(z)\\ \psi_3^{o}(z)\\ \psi_5^{o}(z)\\ \psi_7^{o}(z)\\ \psi_2^{e}(z)\\ \psi_4^{e}(z)\\ \psi_6^{e}(z)\\ \psi_8^{e}(z)\end{bmatrix}.$$

The transition-matrix elements will then be

$$\langle\Phi'_{A}|H'|\Phi_{A}\rangle=\frac{eEP}{2\sqrt{6}\hbar\omega}\{[Z^{A}+(i'\Longleftrightarrow i)]\varepsilon_x+i[Z^{A}-(i'\Longleftrightarrow i)]\varepsilon_y\}\delta(k'_x-k_x)\delta(k'_y-k_y) , \tag{27a}$$

with

$$Z^{A}=\sqrt{3}Z^{e}_{3,1}-Z^{e}_{1,5}+\sqrt{2}Z^{e}_{1,7}+Z^{o}_{6,2}+\sqrt{2}Z^{o}_{8,2}-\sqrt{3}Z^{o}_{2,4}$$

for transitions within the A set;

$$\langle\Phi'_{B}|H'|\Phi_{B}\rangle=\frac{eEP}{2\sqrt{6}\hbar\omega}\{[Z^{B}+(i'\Longleftrightarrow i)]\varepsilon_x+i[Z^{B}-(i'\Longleftrightarrow i)]\varepsilon_y\}\delta(k'_x-k_x)\delta(k'_y-k_y) , \tag{27b}$$

where

$$Z^{B}=\sqrt{3}Z^{o}_{3,1}-Z^{o}_{1,5}+\sqrt{2}Z^{o}_{1,7}+Z^{e}_{6,2}+\sqrt{2}Z^{e}_{8,2}-\sqrt{3}Z^{e}_{2,4} ,$$

for the transitions within the B set, and

$$\langle\Phi'_{B}|H'|\Phi_{A}\rangle=-\frac{eEP}{\sqrt{3}\hbar\omega}[(\sqrt{2}Z^{e}_{2,5}+Z^{e}_{2,7}+\sqrt{2}Z^{e}_{6,1}-Z^{e}_{8,1})$$
$$+(\sqrt{2}Z^{o}_{5,2}+Z^{o}_{7,2}+\sqrt{2}Z^{o}_{1,6}-Z^{o}_{1,8})]\delta(k'_x-k_x)\delta(k'_y-k_y)\varepsilon_z , \tag{27c}$$

for transitions between the A set and the B set. The quantities $Z^{v}_{i',i}$ are defined by Eq. (19), except that in the present case the quantum number n of the Landau levels does not exist. The term $[i'\Longleftrightarrow i]$ stands for the repetition of the preceding term, with i' and i interchanged.

In order to find probable transitions, we must know the components of the wave functions of the states involved. With the discussion in the last section on the subbands and the $\underline{H}_a$, $\underline{H}_b$, and $\underline{H}_c$ given in Ref. 13, we can obtain the significant components of the wave functions for the first two subbands belonging to the conduction band (E series), the light-hole band (lh series), and the heavy-hole band (hh series). In Table I we list the zeroth-order component and the directly coupled components[19] for the first two subbands in each band mentioned above. The coupled components are put into different columns according to the dependence on k_z and $k_\perp$ (the in-plane wave vector) in addition to the components in the column (or columns) on the left.

Since the wave vector of electromagnetic waves is usually in the z direction, we will only discuss transitions allowed by Eqs. (27a) and (27b). Using the zeroth-order

TABLE I. Components of $\underline{F}_A(\mathbf{r})$ and $\underline{F}_B(\mathbf{r})$ for $E1$, $E2$, lh1, lh2, hh1, and hh2 subbands. For both $\underline{F}_A(\mathbf{r})$ and $\underline{F}_B(\mathbf{r})$, the coupled components are listed in columns according to the dependence on k_z and $k_\perp$, in addition to the components in the column (or columns) on the left.

	$\underline{F}_A(\mathbf{r})$			$\underline{F}_B(\mathbf{r})$		
	zeroth order	$k_z\neq 0$ $k_\perp=0$	$k_z\neq 0$ $k_\perp\neq 0$	zeroth order	$k_z\neq 0$ $k_\perp=0$	$k_z\neq 0$ $k_\perp\neq 0$
$E1$	ψ_1^e	ψ_6^o,ψ_8^o	$\psi_3^e,\psi_5^e,\psi_7^e$	ψ_2^e	ψ_5^o,ψ_7^o	$\psi_4^e,\psi_6^e,\psi_8^e$
$E2$	ψ_2^o	ψ_5^e,ψ_7^e	$\psi_4^o,\psi_6^o,\psi_8^o$	ψ_1^o	ψ_6^e,ψ_8^e	$\psi_3^o,\psi_5^o,\psi_7^o$
lh1	ψ_5^e	ψ_2^o	$\psi_1^e,\psi_3^e,\psi_7^e,\psi_4^o$	ψ_6^e	ψ_1^o	$\psi_2^e,\psi_4^e,\psi_8^e\psi_3^o$
lh2	ψ_6^o	ψ_1^e	$\psi_2^o,\psi_4^o,\psi_8^o,\psi_3^e$	ψ_5^o	ψ_2^e	$\psi_1^o,\psi_3^o,\psi_7^o,\psi_4^e$
hh1	ψ_3^e		$\psi_1^e,\psi_5^e,\psi_7^e,\psi_6^o$	ψ_4^e		$\psi_2^e,\psi_6^e,\psi_8^e,\psi_5^o$
hh2	ψ_4^o		$\psi_2^o,\psi_6^o,\psi_8^o,\psi_5^e$	ψ_3^o		$\psi_1^o,\psi_5^o,\psi_7^o,\psi_6^e$

wave functions from Table I in Eqs. (27a) and (27b), we find that the allowed transitions follow the well-known selection rules $\Delta N=0$ (e.g., $E1\rightarrow$lh1). However, k_z is nonvanishing in a superlattice. Furthermore, overlap between wave functions with $\Delta N=\pm 1$ can also occur, as discussed in the preceding section. If $k_\perp$ can be taken as zero while $k_z\neq 0$, the coupled components related to $k_\perp=0$ and $k_z\neq 0$ in Table I have to be included in Eqs. (27a) and (27b). As a result, an additional transition from $E1$ to $E2$ is allowed. When $k_\perp$ has a finite value, in addition to $k_z\neq 0$, all the components listed in Table I should be included, and transitions between *any pair* of the six subbands are in principle possible.

We note finally that there are certain guidelines to follow in estimating the strength of the couplings. For instance, the couplings between the Γ_6 band and the Γ_8 bands are stronger for narrow-gap materials. The couplings between the different Γ_8 bands are only present if $k_\perp\neq 0$. With these couplings considered, the selection rule $\Delta N=0$ has to be changed to $\Delta N=0,\pm 1$, which is more important if narrow-gap materials are involved. This is consistent with the numerical calculations in the tight-binding scheme presented in Ref. 20. It can be shown, in the same way, that such a change in the selection rules is also necessary for higher subbands.

V. CONCLUDING REMARKS

Although Fig. 1 represents the simplest case of a type-I superlattice, the results apply equally well to type-II and -III superlattices. Furthermore, the results can also be used for cases where band bending occurs because of electrons and holes transferring between neighboring layers. The only requirements for the above-selection rules to be valid are that the band bending is symmetric around the center of each layer, and that the states in question are not the ones trapped at the interfaces by the band bending itself (in which case the envelope-function approximation used here may be inappropriate).

In fact, with all the assumptions made, the validity of the results described above can be generally stated as follows: the results can be applied to any layered structure consisting of zinc-blende materials in which the basis functions, $u_i(\mathbf{r})$, are approximately the same for all the materials and the $\mathbf{k}\cdot\mathbf{p}$ approximation can be used, and a plane can be found through which the system is symmetric under a reflection R. One finds that a single square quantum well made of CdTe and HgTe with a width much larger than the lattice parameter of the material satisfies such requirements. One can also find other systems which meet these assumptions.

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