Exact symmetries of electron Bloch states and optical selection rules in [001] GaAs/AlAs quantum wells and superlattices

P. Tronc* and Yu. E. Kitaev†
Laboratoire d'Optique Physique, Ecole Superieure de Physique et Chimie Industrielles, 10 rue Vauquelin, 75005 Paris, France
(Received 25 July 2000; published 7 May 2001)

We determined the exact symmetries of conduction and valence Bloch states in type-I and type-II [001] $(GaAs)_m(AlAs)_n$ superlattices at the Γ point and at some other symmetry points of the Brillouin zone of the superlattices and derived optical selection rules. Contrary to a result widely accepted in the envelope-function approximation (EFA), p_z atomic orbitals cannot mix with p_x and p_y orbitals to build Bloch states. The phonon-assisted transitions involving the Γ point as an initial or final state are allowed both without and with taking into account the spin-orbit interaction whatever are the symmetries of the initial and final states. The electron band structure of the superlattices is discussed. Within the domain of validity of EFA (i.e., for not too small values of m and n), a detailed analysis of the Bloch-state symmetry and selection rules is provided on imposing invariance of the superlattice structure under the change of z to $-z$ (the σ_z symmetry operation). It is shown that optical transitions between the conduction states arising from the Γ states of GaAs on one hand and the conduction states arising from the X states of AlAs on the other hand can be allowed from spin-orbit coupling only. The correspondence is provided between the symmetry of a Bloch state and the parity with respect to σ_z of its associated envelope function. The effect of an electric field parallel to the growth axis is discussed. Quantum wells do not differ from superlattices with regard to Bloch-state and envelope-function symmetries or optical selection rules. All the above results are still valid for any pseudomorphic superlattice or quantum well made of two binary compounds with zinc-blend structure and identical cations or anions, such as, for example, in the GaN/AlN system.

DOI: 10.1103/PhysRevB.63.205326 PACS number(s): 78.66.−w

I. INTRODUCTION

The space groups of the [001] $(GaAs)_m(AlAs)_n$ superlattices (SL's) have been shown to be D_{2d}^5 for the even values of $m+n$ and D_{2d}^9 for the odd ones.[1] Using a group-theory method based on site-symmetry analysis, we determined[2] the possible exact symmetries of extended electron states (Bloch states) and their symmetry relation with localized s and p atomic orbitals at the Γ point and at the other symmetry points of the superlattice Brillouin zone (SLBZ). Among these other points, we consider hereafter the Z and X points of SL's with the D_{2d}^5 space group and the M and X points of SL's with the D_{2d}^9 one. These points are of particular interest since they are located at the surface of the SLBZ in directions parallel and perpendicular to the growth axis, respectively.[2] Hereafter, the point group irreducible representations (irreps) are labeled according to Ref. 3 and the labeling of space group irreps follows Ref. 4.

We start our study by focusing on the case where spin-orbit coupling is not taken into account, thus putting the emphasis on the most important features of optical spectra. At the Γ point, in the case when spin-orbit coupling is not taken into account the possible symmetries for Bloch states[2] are Γ_1,Γ_2 (both generated by s and p_z orbitals of constituent atoms), and Γ_5 (generated by p_x and p_y orbitals). The Γ_3 and Γ_4 symmetries are possible only for free excitons. The $Z(M)$ point of SLBZ has the same symmetry (D_{2d}) as the Γ point. It makes the possible symmetries for Bloch states to be $Z_1(M_1)$ and $Z_2(M_2)$, both generated by s and p_z orbitals, and $Z_5(M_5)$, generated by p_x and p_y orbitals. Finally, at the X point of SLBZ, s and p orbitals can induce states with any symmetry (X_{1-4}). These results from our model are valid whatever are the n and m values since only the number of atoms in the lattice with C_{2v} site symmetry and their z coordinates can vary with m and n.[2]

The selection rules for direct optical transitions that we derived extensively in Ref. 2 are the same at the Γ (Table I) and $Z(M)$ points since they have the same D_{2d} symmetry. The situation is more complicated at the X point. Indeed, whereas the Bloch-state symmetry and optical selection rules are governed by the point group at the Γ point and at the SLBZ points with the same highest symmetry [among them, the $Z(M)$ point in the present case], the property does not hold at the other SLBZ points. The space group has then to be taken into account. It can be seen that the two families of SL's differ from one another in several respects at the X point: (i) the X point in D_{2d}^5 SL's has the C_{2v} symmetry whereas it has the D_2 one in D_{2d}^9 SL's; (ii) in the z polariza-

TABLE I. The selection rules for direct band-to-band optical transitions at the Γ point of SL's with the D_{2d}^5 and D_{2d}^9 space groups. The labels of the irreps taken in brackets refer to the case when the spin-orbit interaction is not taken into account. Polarizations in parentheses refer to transitions allowed only with including the spin-orbit interaction; the ones in capitals refer to transitions allowed in any case.

	$\Gamma_6[\Gamma_1]$	$\Gamma_7[\Gamma_2]$	$\Gamma_6[\Gamma_5]$	$\Gamma_7[\Gamma_5]$
$\Gamma_6[\Gamma_1]$	(x,y)	$(x,y)Z$	X,Y	$X,Y(z)$
$\Gamma_7[\Gamma_2]$	$(x,y)Z$	(x,y)	$X,Y(z)$	X,Y
$\Gamma_6[\Gamma_5]$	X,Y	$X,Y(z)$	(x,y)	$(x,y)Z$
$\Gamma_7[\Gamma_5]$	$X,Y(z)$	X,Y	$(x,y)Z$	(x,y)

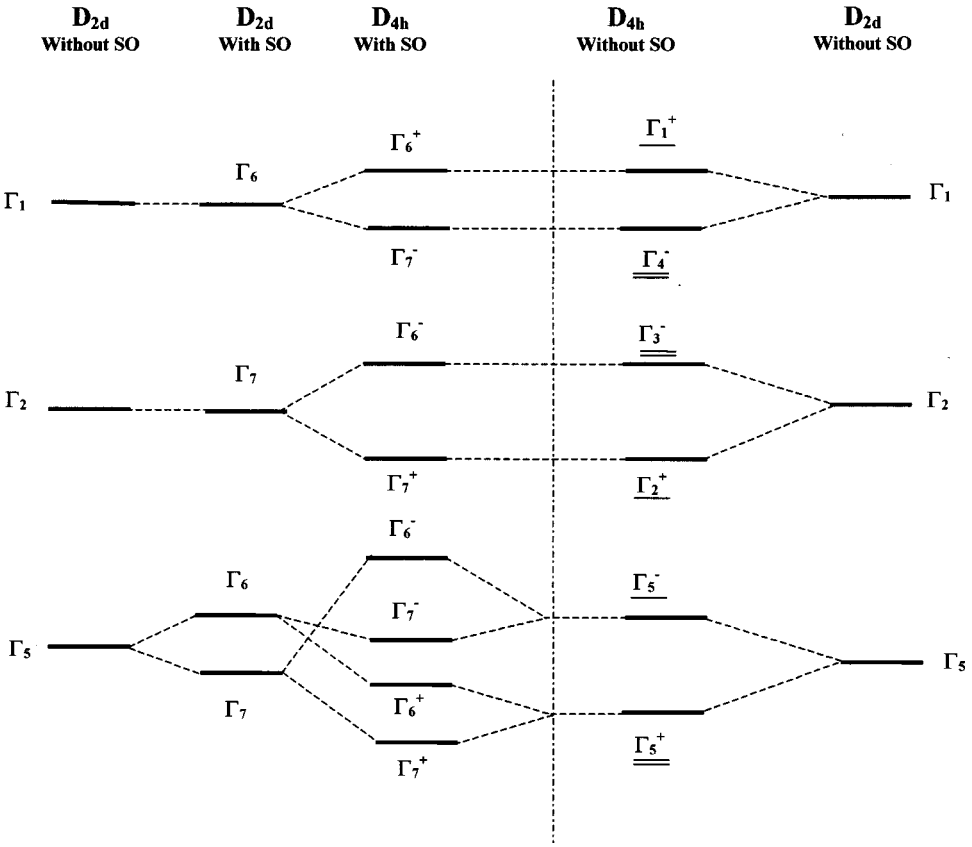

FIG. 1. Subduction of irreps of the D_{4h} group on the D_{2d} group without (right side) and with (left side) the account of the spin-orbit interaction. The correspondence between single- and double-valued irreps is shown. The parity with respect to z of the associated envelope functions is indicated by one (two) bar(s) below the irrep symbol for even (odd) character.

tion, direct transitions between two X states with the same index (X_{1-4}) are forbidden in the D_{2d}^9 SL's, whereas they are allowed in the D_{2d}^5 SL's (note that the X irreps refer to the C_{2v} group in D_{2d}^5 SL's and to the D_2 group in D_{2d}^9 SL's); (iii) in the (x,y) polarization, the selection rules obey the relations with the same indices in both families of SL's, direct transitions being allowed from X_1 and X_2 states to X_3 and X_4 ones.[2]

When spin-orbit coupling is taken into account,[2] Γ_1 is transformed into Γ_6, Γ_2 into Γ_7, and Γ_5 is split into Γ_6 and Γ_7 (Fig. 1). Any transition previously forbidden in the (x,y) polarization becomes weakly allowed (Table I). In the z polarization, a transition between a $\Gamma_6(\Gamma_7)$ state arising from Γ_5 on one hand and a $\Gamma_7(\Gamma_6)$ state arising from $\Gamma_2(\Gamma_1)$ on the other hand also becomes weakly allowed from spin-orbit coupling. The same transformations of irreps and modifications of selection rules are induced by spin-orbit coupling at the $Z(M)$ point. At the X point, there is only one double-valued irrep X_5 for both families of SL's. Any transition becomes allowed in any polarization. Of course, transitions allowed from spin-orbit interaction only are expected to have weak intensities. The experiments with light polarized in the (x,y) plane are particularly important since they are easier to perform than those in the z polarization (light propagating along the z axis can be used in the former case).

Finally, it should be mentioned that any phonon-assisted transition between the Γ point and the Z or X point of SL's with the D_{2d}^5 space group (the M and X point of SL's with the D_{2d}^9 space group) is allowed both without and with taking into account the spin-orbit interaction and whatever are the symmetries of the involved initial and final states.[2]

II. EXACT SYMMETRIES OF BLOCH FUNCTIONS AT THE Γ POINT

It is widely accepted that the lowest conduction band is built from s orbitals at the Γ point of bulk GaAs, whereas the upper valence bands originate from p orbitals and present a pronounced maximum in energy at this point. It is therefore reasonable to assume that the maximum in energy for upper valence bands in SL's is located at the Γ point of SLBZ. Bulk AlAs is an indirect-gap semiconductor with the minimal energy value in the lowest conduction band lying at the X points of BZ, the corresponding Bloch states being built from s and p orbitals.[5] The SL's have generally been studied using the envelope-function approximation (EFA) and starting from properties of bulk GaAs and AlAs. Within EFA, it is generally accepted that the lowest conduction Bloch in type-II SL's states originate from X states of AlAs slabs: either the X_z state or the X_x and X_y states depending on the n and m values.[6] Besides, within EFA, the heavy-hole Bloch states at the Γ point of SLBZ are assumed to be built from p_x and p_y orbitals only whereas the light- and spin-orbit-split-off-hole Bloch states are built from the three p orbitals.[7] The assumption that p_z orbitals contribute to light- and split-off-hole Bloch states makes the optical transition to the conduction band allowed in the z polarization. To our knowledge, this last prediction has never been experimentally verified.

On the contrary, our results show that p_z orbitals cannot mix at the Γ point with p_x and p_y ones since they induce

Bloch states with different symmetries.[2] Our theory allows us to assign, as possible exact symmetries in the vicinity of band gap, the Γ_1 and Γ_2 symmetries for conduction states arising from s and p_z orbitals and the Γ_5 symmetry for heavy-, light-, and split-off-hole states arising from p_x and p_y orbitals. We assume the conduction states arising from p_x and p_y orbitals (their possible symmetry is Γ_5) to be higher in energy and the hole states originating from s and p_z orbitals (their possible symmetries are Γ_1 and Γ_2) to be lower. These assignments arise from comparison between widely experimentally checked selection rules and predictions from our theory. Indeed, experiments show that interband transitions are allowed only in the (x,y) polarization, whereas intraband transitions are allowed only in the z polarization. Correlatively, our theory[2] states that, in the (x,y) polarization, only the transitions between Γ_5 on one hand and Γ_1 or Γ_2 on the other hand are allowed whereas, in the z polarization, the allowed transitions take place between Γ_1 and Γ_2 or between two Γ_5 only (Table I). Finally, when spin-orbit coupling is taken into account, the possible symmetries are Γ_6 and Γ_7 for both the conduction and valence states (see Sec. I).

The$(\mathrm{GaAs})_m(\mathrm{AlAs})_n$ SL's are generally grown on GaAs substrates. The difference in lattice parameter between GaAs and AlAs crystals induces a strain in AlAs slabs only, making the AlAs lattice parameter slightly larger in the z direction [it is equal to that of GaAs in the (x,y) plane]. This changes neither the point symmetry of the SL's nor their space symmetry. Moreover, atoms with the D_{2d} site symmetry undergo no change since they are located at the center of the slabs[2,8] and atoms with the C_{2v} site symmetry may vary their z coordinate.[2] Therefore any orbital of any atom induces Bloch states with the same symmetries as in the no-strain case. The strain can only change the energy of bands and the relative contributions of atoms to the Bloch states. Note that the difference in energy between conduction states arising (according to the EFA picture) from the $X_{x,y}$ and X_z points of AlAs BZ, has been experimentally shown to be 19 meV in type-II SL's when confinement energy is not taken into account.[6]

III. COMPARISON WITH THE ENVELOPE-FUNCTION APPROXIMATION

EFA has been shown to be, in many respects, a very useful tool to study electron states in SL's except perhaps in the cases where very thin layers (of the order of a few monolayers) are involved. We try to determine hereafter how the results from EFA can be compared with those from our theory. In EFA, any plane perpendicular to the growth axis and located at the center of any slab is imposed as a symmetry plane for the structure. However, in fact, these symmetry planes do exist at a microscopic level neither for the D_{2d}^5 nor for the D_{2d}^9 space group. When introducing the (x,y)-symmetry plane (hereafter referred to as the σ_z symmetry operation), the point group of the structure is transformed from D_{2d} into D_{4h}. As a result, the number of symmetry elements becomes 16 (including inversion) instead of 8. The D_{4h} group is the direct product of the D_{2d} group and the C_s group (the C_s group consists of identity and σ_z operations)

$$D_{4h}=D_{2d}\times C_s. \tag{1}$$

In the same manner, the space groups are transformed as follows:

$$D_{2d}^5\times C_s=D_{4h}^1,\quad D_{2d}^9\times C_s=D_{4h}^{17}. \tag{2}$$

The irreps of the D_{4h} point group can be combined into pairs. Within each pair, one irrep can be labeled with $+$ and the other with $-$. The associated Γ states are, respectively, even and odd under inversion. Of course, the larger the m and n values, the better the approximation, since the details of the microscopic structure become less and less significant. Correlatively, it is expected that for not too small values of m and n, Γ irreps of the D_{2d} group present symmetry properties close to those of Γ irreps of the D_{4h} group. Thus, all the Γ states of the D_{2d} group corresponding to a given one-dimensional irrep (i.e., Γ_1 or Γ_2) should present the same approximate parity with respect to inversion. They should also present the same approximate parity with respect to σ_z. Note that these two parities may be different. To find a correspondence between the irreps of the D_{2d} and D_{4h} groups, one should subduce the irreps of the D_{4h} group onto its D_{2d} subgroup.

A. The spin-orbit interaction not being taken into account

The subduction procedure provides the following correspondences between Γ irreps of the D_{4h} and D_{2d} groups (Fig. 1):

$$\Gamma_1^+,\Gamma_4^-\rightarrow\Gamma_1,\quad \Gamma_3^-,\Gamma_2^+\rightarrow\Gamma_2,\quad \Gamma_5^+,\Gamma_5^-\rightarrow\Gamma_5. \tag{3}$$

The irreps Γ_{1-4}^+ are one-dimensional and the irreps $\Gamma_5^\pm$ are two-dimensional. The irreps Γ_1^+, Γ_2^+, and Γ_5^- are even with respect to σ_z whereas the Γ_3^-, Γ_4^-, and Γ_5^+ irreps are odd.[4] The subduction procedure, from the point of view of symmetry, mixes states that previously had opposite parities with respect to σ_z, namely, Γ_1^+ and Γ_4^- as well as Γ_3^- and Γ_2^+. It occurs because Γ_1 and Γ_2 have no defined parity with respect to σ_z. Now we can draw conclusions on conduction electron states based on selection rules. The vector representation for the D_{4h} group is $\Gamma_5^-(x,y)+\Gamma_3^-(z)$. Of course, the vector representation that is odd with respect to inversion can only connect states of opposite parities with respect to this transformation. The selection rules for direct optical transitions between the states with Γ_1^+, Γ_3^-, and Γ_5^- symmetries are the same as those between the states with Γ_4^-, Γ_2^+, and Γ_5^+ symmetries, respectively. No transition is allowed between Γ_1^+ (or Γ_3^-) and Γ_4^- (or Γ_2^+) (Table II). Finally, the selection rules between Γ_1^+, Γ_3^-, and $\Gamma_5^+ + \Gamma_5^-$, as well as between Γ_4^-, Γ_2^+, and $\Gamma_5^- + \Gamma_5^+$, are the same as those between Γ_1, Γ_3^-, and Γ_5 irreps of the D_{2d} group[2] (Table I). This shows that there are two sets of possible approximate symmetries for conduction electrons at the Γ point, one being Γ_1^+ and Γ_3^-, the other Γ_4^- and Γ_2^+. Each set presents one even and one odd possible symmetries with respect to σ_z. Transitions between the two sets are forbidden even in the z polarization whatever are the parities with respect to σ_z of

TABLE II. The selection rules for direct band-to-band optical transitions at the Γ point of SL's with the D_{4h} point symmetry (without including the spin-orbit interaction).

	Γ_1^+	Γ_3^-	Γ_5^-	Γ_4^-	Γ_2^+	Γ_5^+
Γ_1^+		z	x,y			
Γ_3^-	z					x,y
Γ_5^-	x,y				x,y	z
Γ_4^-					z	x,y
Γ_2^+			x,y	z		
Γ_5^+		x,y	z	x,y		

the two states considered for a transition. Both sets of possible approximate symmetries therefore cannot be assigned to the same type of electron state. For lower energy-conduction bands, we assign one set to electrons originating from Γ states in GaAs (in the EFA picture) and the other set to electrons originating from *X* states in AlAs. The GaAs and AlAs slabs play the same role from the point of view of symmetry, therefore both sets of electrons differ only in symmetry properties by a half-SL-period translation along the *z* axis. The assignment of a set of symmetries to a set of electrons depends only on the choice of origin on the *z* axis (in the center of a GaAs or AlAs slab).

As the Γ Bloch states in the D_{4h} groups have a defined parity with respect to inversion, it follows that the associated envelope functions should also have this property. Thus, the question arises of the relation between the parity with respect to σ_z of a Bloch wave function and the parity of the corresponding envelope function in SL's. It is widely known from selection rules predicted in EFA (Ref. 7) and verified experimentally that interband (intraband) transitions are forbidden between states whose envelope functions have the opposite (the same) parities with respect to σ_z. Obviously, an even Bloch function (Γ_1^+, Γ_2^+, or Γ_5^-) can correspond to an even envelope function only. Furthermore, considering the selection rules displayed in Table II within each set of conduction states and between each set of conduction states and valence states, one must conclude that the envelope functions associated with Γ_3^-, Γ_4^-, and Γ_5^+ Bloch states are odd with respect to σ_z. Therefore, in EFA, a Bloch state and its associated envelope function have the same parity with respect to σ_z. The results appear in Fig. 1. Moreover, it can be deduced from experiment that Γ conduction states, at least in type I SL's for which numerous experimental results have been published, present alternatively even or odd symmetries with increasing values of energy.

B. The spin-orbit interaction being taken into account

The double-valued irreps of the D_{4h} group have a defined parity with respect to inversion and may also be labeled with a + or − index. Unlike single-valued irreps, double-valued irreps have no defined parity with respect to σ_z (this arises from the rotation of the spin). Nevertheless, the spin-orbit interaction being only of a perturbative order of magnitude, it is probably a good approximation to assume that the symmetry properties of double-valued irreps of the D_{4h} group with respect to σ_z remain approximately the same as those of single-valued irreps from which they originate. It is noted that EFA also does take into account the spin-orbit interaction[7] and provides envelope functions with a defined parity with respect to σ_z.

TABLE III. The selection rules for direct band-to-band optical transitions at the Γ point of SL's with the D_{4h} point symmetry (with including the spin-orbit interaction).

	Γ_6^+	Γ_6^-	Γ_7^-	Γ_7^+
Γ_6^+		x,y,z	x,y	
Γ_6^-	x,y,z			x,y
Γ_7^-	x,y			x,y,z
Γ_7^+		x,y	x,y,z	

The spinor irrep in the D_{4h} groups is Γ_6^+. When the spin-orbit interaction is taken into account, the subduction of irreps of the D_{4h} group onto its D_{2d} subgroup provides the following correspondences (Fig. 1):

$$\Gamma_6^+,\Gamma_7^-\rightarrow\Gamma_6, \quad \Gamma_6^-,\Gamma_7^+\rightarrow\Gamma_7. \tag{4}$$

Besides, the correspondences between the single- and double-valued irreps of the D_{4h} group are (Fig. 1):

$$\Gamma_1^+\rightarrow\Gamma_6^+, \quad \Gamma_4^-\rightarrow\Gamma_7^-, \quad \Gamma_3^-\rightarrow\Gamma_6^-, \quad \Gamma_2^+\rightarrow\Gamma_7^+, \tag{5}$$

$$\Gamma_5^+\rightarrow\Gamma_6^+ + \Gamma_7^+, \quad \Gamma_5^-\rightarrow\Gamma_6^- + \Gamma_7^-.$$

Therefore, the two sets of conduction states mentioned above have the Γ_6^+ and Γ_6^- symmetries and the Γ_7^- and Γ_7^+ symmetries, respectively. The possible symmetries for valence states are Γ_6^+, Γ_6^-, Γ_7^+, and Γ_7^-. As mentioned above, it is probably a good approximation to assume that Γ_6^+ and Γ_7^+ are even with respect to σ_z as they originate from Γ_1^+ and Γ_2^+, respectively, whereas Γ_6^- and Γ_7^- are odd as they originate from Γ_3^- and Γ_4^-, respectively. The former states would then correspond to even envelope functions and the latter states to odd ones. The selection rules are listed in Table III. We now deal with the two sets of conduction states. In Table IV, to provide a presentation of results corresponding to that of Table II, the contributions of Γ_6^- and Γ_7^- irreps arising from Γ_5^- have been added, as well as those of Γ_6^+ and Γ_7^+ irreps arising from Γ_5^+. It can be seen that transitions become weakly allowed in the (x,y) polarization between two states belonging to different sets of conduction states when they have opposite parities with respect to inversion but transitions remain forbidden in all cases in the *z* polarization. Next, the selection rules between Γ_6^+, Γ_6^-, and $\Gamma_6^+ + \Gamma_6^- + \Gamma_7^- + \Gamma_7^+$, as well as between Γ_7^-, Γ_7^+, and $\Gamma_6^+ + \Gamma_6^- + \Gamma_7^- + \Gamma_7^+$, are identical. They are close to those between Γ_6, Γ_7, and $\Gamma_6 + \Gamma_7$ of the D_{2d} group[2] (Table I). The only difference is that transitions between two states with the same symmetry (Γ_6 or Γ_7) is weakly allowed in the D_{2d} group from spin-orbit interaction[2] (Table I) whereas they are forbidden in the D_{4h} group as any state there has a defined parity with respect to inversion (Table III). The difference

TABLE IV. The selection rules for direct band-to-band optical transitions at the Γ point of SL's with the D_{4h} point symmetry. The notations are the same as in Table I.

	$\Gamma_6^+[\Gamma_1^+]$	$\Gamma_6^-[\Gamma_3^-]$	$(\Gamma_6^-+\Gamma_7^-)[\Gamma_5^-]$	$\Gamma_7^-[\Gamma_4^-]$	$\Gamma_7^+[\Gamma_2^+]$	$(\Gamma_6^++\Gamma_7^+)[\Gamma_5^+]$
$\Gamma_6^+[\Gamma_1^+]$		$(x,y)Z$	$X,Y(z)$	(x,y)		
$\Gamma_6^-[\Gamma_3^-]$	$(x,y)Z$				(x,y)	$X,Y(z)$
$(\Gamma_6^-+\Gamma_7^-)[\Gamma_5^-]$	$X,Y(z)$				$X,Y(z)$	$(x,y)Z$
$\Gamma_7^-[\Gamma_4^-]$	(x,y)				$(x,y)Z$	$X,Y(z)$
$\Gamma_7^+[\Gamma_2^+]$		(x,y)	$X,Y(z)$	$(x,y)Z$		
$(\Gamma_6^++\Gamma_7^+)[\Gamma_5^+]$		$X,Y(z)$	$(x,y)Z$	$X,Y(z)$		

arises from the σ_z element that is imposed in EFA. The existence of two sets of possible approximate symmetries for conduction states at the Γ point, namely, Γ_6^+ and Γ_6^- on one hand and Γ_7^- and Γ_7^+ on the other hand is thus confirmed. Finally, if one assumes that an approximate parity with respect to σ_z can be assigned to double-valued irreps, comparing Eqs. (4) and (5) draws the conclusion that the ground state of hole of any type (heavy, light or split-off) or electron (belonging to either of the two sets) can have only the Γ_6^+ or the Γ_7^+ symmetry since in EFA the ground state is always associated with an even envelope function.

To conclude, it must be stressed that the main feature of EFA consists of imposing the σ_z symmetry on the structure of SL's. In addition, both barriers and wells in EFA are assumed to be made of materials completely defined by the values of the band gap and the carrier-effective masses. On the contrary, when introducing the σ_z symmetry in our theory, we kept all symmetry elements of the D_{2d}^5 or D_{2d}^9 space group. These elements are not included in the crude assumptions of EFA. As a result, we may expect some discrepancies between EFA and our model even after adding to the latter the invariance with respect to σ_z. For example, we found that any optical transition at the Γ point of SLBZ is forbidden in the *z* polarization between the two sets of conduction states. This property is not a feature of EFA where intraband transitions between states with envelope functions of opposite parities with respect to σ_z are allowed[7] in the *z* polarization.

IV. BAND STRUCTURE

A. Γ-$Z(M)$ bands

To study the symmetry behavior of electron bands, one should determine which atoms in the primitive cell of the SL's mainly contribute to them. The only atoms with D_{2d} site symmetry in any SL are those located at the center of each slab (GaAs or AlAs).[2,8] The influence of such atoms on electron band structure and optical properties of SL's therefore decreases as the thickness of the slabs is increased. For other atoms (all of them have the C_{2v} site symmetry), when the spin-orbit interaction is not taken into account, any orbital (s,p_x,p_y,p_z) induces Γ and $Z(M)$ Bloch states with the same possible symmetries.[2] Note that this result also holds when one takes into account the atoms with the D_{2d} site symmetry that are located at the $1a$ Wyckoff position in both space groups. For the other atoms with the D_{2d} site symmetry ($1c$ and $1d$ Wyckoff positions in the D_{2d}^5 space group and $1c$ in the D_{2d}^9 group), *s* and p_z orbitals exchange the indices of the Bloch states they induce when going from the Γ point to the $Z(M)$ point.

In EFA, using a tight-binding model and considering direct optical transitions in the (x,y) polarization,[9] it has been shown that a type I allowed (forbidden) transition at the Γ point is also allowed (forbidden) at the *Z* or *M* point of the same miniband. On the contrary, for a type-II transition of an electron originating from the X_z point of bulk AlAs, the characters are opposite at each end of the miniband. This result arises from the spatial configuration of electron and hole envelope functions. The parity of envelope functions under the σ_z operation is the same at the Γ and $Z(M)$ points.[9]

In our model, compatibility relations[4] show that within the same miniband, Γ_1 and Γ_2 can be in correspondence with both $Z_1(M_1)$ and $Z_2(M_2)$ and Γ_5 in correspondence with $Z_5(M_5)$. The symmetry properties of the $Z_1(M_1)$, $Z_2(M_2)$, and $Z_5(M_5)$ irreps are the same as those of the Γ_1, Γ_2, and Γ_5 irreps, respectively, and they therefore obey the same selection rules. It can be concluded that type-I transitions correspond to $\Gamma_1-Z_1(M_1)$ or $\Gamma_2-Z_2(M_2)$ minibands whereas type-II transitions correspond to $\Gamma_1-Z_2(M_2)$ or $\Gamma_2-Z_1(M_1)$ minibands. When the spin-orbit interaction is taken into account, atoms with either the D_{2d} or C_{2v} site symmetry can induce Bloch states with any possible symmetry at the Γ and $Z(M)$ points. Compatibility relations[4] show that, within the same miniband, Γ_6 and Γ_7 can be in correspondence with both $Z_6(M_6)$ and $Z_7(M_7)$. The symmetry properties of $Z_6(M_6)$ and $Z_7(M_7)$ are the same as those of Γ_6 and Γ_7, respectively, and they obey the same selection rules. As above, it can be concluded that type-I transitions correspond to $\Gamma_6-Z_6(M_6)$ or $\Gamma_7-Z_7(M_7)$ minibands whereas type-II transitions correspond to $\Gamma_6-Z_7(M_7)$ or $\Gamma_7-Z_6(M_6)$ minibands.

B. Γ-*X* bands

The *X* point of SLBZ has different symmetry properties in each family of SL's (see Sec. I). When the spin-orbit interaction is not taken into account, atoms with either the D_{2d} or C_{2v} site symmetry can induce Bloch states with any possible symmetry. Compatibility relations[4] show that, in D_{2d}^5 SL's, Γ_1 and Γ_2 can be, within the same miniband, in correspondence with X_1 and X_3, and Γ_5 with X_{1-4}, whereas in D_{2d}^9 SL's, Γ_1 is in correspondence with X_1 and X_3, Γ_2 with X_2

and X_4, and Γ_5 with X_{1-4}. Obviously, for sufficiently large values of m and n, the optical properties of each family should converge to one another. Nevertheless, it is difficult to make predictions about these properties due to the complexity of the situation, in particular, the fact that a Γ_5 state can be in correspondence with an X state with any possible symmetry (X_{1-4}) within the same valence miniband. When the spin-orbit interaction is taken into account, any Bloch state at the X point of the SLBZ has the X_5 symmetry and can be in correspondence within a miniband either with a Γ_6 or Γ_7 state.[4]

Band-structure predictions should possibly be modified in the case of band crossings since these could modify the symmetry correspondence between the points at each end of the miniband.

V. EFFECT OF AN ELECTRIC FIELD

Application of an electric field along the z direction lifts the SL translational invariance along the growth axis. [This statement could not be true in the special case of a SL with a periodic field, embedded in a structure presenting the same type of doping at both ends and/or submitted to an applied voltage. Periodic fields can arise from the difference in lattice parameter between the well and barrier materials (piezoelectric field) or from difference in spontaneous polarizability.[10] Periodic fields are forbidden from symmetry in the present SL's and we therefore do not consider this case.] The full symmetry is kept in the (x,y) plane. The electric field removes the S_4 symmetry elements as well as the two-fold symmetry axes lying in the (x,y) plane. The point group becomes C_{2v}, a subgroup of the D_{2d} point group of the SL when no field is applied ($D_{2d}=C_{2v}\times S_4$, where the S_4 group consists of identity and S_4 along the z axis operations). The space symmetry of the structure is then described by the three-dimensional diperiodic space group (layer group) DG23 ($P2mm$). The diperiodic groups (DG's) referred to in the present paper follow the notations of Wood.[11] The 2D BZ of the DG is the cross-section ($k_z=0$) of the 3D BZ of the corresponding 3D group. The states from the symmetry lines parallel to the k_z axis are projected onto the (k_x,k_y) plane. This causes, for example, the $Z(M)$ point of SLBZ to be located at the Γ point whereas the X point of SLBZ remains in the same location. In the present case, the x and y axes are no longer equivalent. The subduction procedure provides the following correspondences between the Γ irreps of the D_{2d} and C_{2v} groups, respectively, when the spin-orbit is not taken into account [see Eq. (6)] and when it is [see Eq. (7)]:

$$\Gamma_1,\Gamma_2\rightarrow\Gamma_1, \quad \Gamma_5\rightarrow\Gamma_3+\Gamma_4, \tag{6}$$

$$\Gamma_6,\Gamma_7\rightarrow\Gamma_5. \tag{7}$$

The splitting of Γ_5 into Γ_3 and Γ_4 arises from the nonequivalence of the x and y axes in the C_{2v} group.

When adding the σ_z symmetry operation (EFA), the point group becomes C_{4v}, a subgroup of D_{4h} ($D_{4h}=C_{4v}\times C_s$), and the three-dimensional diperiodic space group becomes DG55 ($P4mm$). The four-fold symmetry axis is kept in addition to the two vertical symmetry planes. Such results are in agreement with properties previously obtained when studying the valence-band structure of quantum wells (QW's) under an electric field.[12]

TABLE V. The selection rules for direct band-to-band optical transitions at the Γ point of SL's with the C_{2v} point group. The notations are the same as in Table I.

	$\Gamma_5[\Gamma_1]$	$\Gamma_5[\Gamma_3]$	$\Gamma_5[\Gamma_4]$
$\Gamma_5[\Gamma_1]$	$(x,y)Z$	$(x)Y(z)$	$X(y,z)$
$\Gamma_5[\Gamma_3]$	$(x)Y(z)$	$(x,y)Z$	(x,y,z)
$\Gamma_5[\Gamma_4]$	$X(y,z)$	(x,y,z)	$(x,y)Z$

The subduction procedure provides the following correspondences between the Γ irreps of the D_{4h} and C_{4v} groups when spin-orbit is not taken into account [see Eq. (8)] and when it is [see Eq. (9)]:

$$\Gamma_1^+,\Gamma_3^-\rightarrow\Gamma_1, \quad \Gamma_4^-,\Gamma_2^+\rightarrow\Gamma_2, \quad \Gamma_5^+,\Gamma_5^-\rightarrow\Gamma_5, \tag{8}$$

$$\Gamma_6^+,\Gamma_6^-\rightarrow\Gamma_7, \quad \Gamma_7^+,\Gamma_7^-\rightarrow\Gamma_6. \tag{9}$$

It can be seen that there are no longer two separate sets of conduction-electron states. Indeed, due to the electric field, the GaAs and AlAs slabs no longer play equivalent roles from the symmetry point of view. The electric field mixes states that previously had opposite parities with respect to σ_z (Γ_1^+ and Γ_3^- on one hand and Γ_4^- and Γ_2^+ on the other hand when the spin-orbit is not taken into account, and Γ_6^+ and Γ_6^- as well as Γ_7^+ and Γ_7^- when it is). Of course, any Bloch state or envelope function no longer has a defined parity with respect to σ_z as the C_{4v} group does not include the σ_z symmetry operation. Such a result has been shown directly for envelope functions in the case of the Wannier-Stark effect.[13]

The optical selection rules for direct transitions at the Γ point are given in Table V for the C_{2v} group.[14] Those for the C_{4v} group are given in Table VI (the spinor irrep is Γ_7). The possible symmetries in the C_{2v} (C_{4v}) group are Γ_1 (Γ_1 and Γ_2) for conduction states and Γ_3 and Γ_4 (Γ_5) for valence states. These assignments arise from the above subduction procedures. In the x and y polarizations, for both groups, direct transitions between conduction and valence states remain fully allowed (both without and with the account of the spin orbit), just as they were when no electric field was ap-

TABLE VI. The selection rules for direct band-to-band optical transitions at the Γ point of SL's with the C_{4v} point group. The notations are the same as in Table I. Polarizations in brackets refer to transitions allowed only without including the spin-orbit interaction.

	$\Gamma_7[\Gamma_1]$	$\Gamma_6[\Gamma_2]$	$\Gamma_6[\Gamma_5]$	$\Gamma_7[\Gamma_5]$
$\Gamma_7[\Gamma_1]$	$(x,y)Z$	(x,y)	X,Y	$X,Y(z)$
$\Gamma_6[\Gamma_2]$	(x,y)	$(x,y)Z$	$X,Y(z)$	X,Y
$\Gamma_6[\Gamma_5]$	X,Y	$X,Y(z)$	$(x,y)Z$	$(x,y)[z]$
$\Gamma_7[\Gamma_5]$	$X,Y(z)$	X,Y	$(x,y)[z]$	$(x,y)Z$

plied. Only, the x and y polarizations can now be distinguished from one another in the C_{2v} group due to the splitting of valence bands into Γ_3 and Γ_4 components. In the z polarization, on the contrary, for both groups the transitions are fully allowed between states with the same symmetry, whereas they were previously forbidden both without and with the account of the spin-orbit. Moreover, in the z polarization, transitions between conduction (valence) states with different symmetries were previously fully allowed. They are now allowed in the C_{2v} group from the spin-orbit only between valence states (there is only one possible symmetry for conduction states). In the C_{4v} group, they are allowed only without the account of spin-orbit between valence states, and are completely forbidden between conduction states. This arises because the electric field lifts the symmetry operations involving the transformation of z in $-z$, namely, the S_4 operations, the two two-fold symmetry axes lying in the (x,y) plane, and in addition the σ_z mirror symmetry for the D_{4h} group.

It should be kept in mind that in some cases, for example, in the case of a uniform applied electric field (the Wannier-Stark effect[15,16]), the extension of the wave function along the z direction can be limited. Independently of the above selection rules, which arise from symmetry, this limitation can also cause the matrix elements to vanish when the electron and the hole are located far from one another in the z direction.

VI. QUANTUM WELLS

We have previously shown[8] that the point group and the three-dimensional diperiodic space group of [001] $(GaAs)_m/AlAs$ OW's are D_{2d} and DG 59 ($P\bar{4}m2$), respectively, whatever is the m value (of course, an identical picture would be obtained with AlAs by merely replacing m with n). When an electric field is applied parallel to the growth axis, these groups transform into C_{2v} and DG23 ($P2mm$), respectively. When adding the σ_z symmetry operation (EFA), they transform into D_{4h} and DG61 ($P4/mmm$), respectively, when the electric field is not applied and C_{4v} and DG55 ($P4mm$), respectively, when the field is applied. At corresponding points of BZ (see Sec. V), the possible symmetries for conduction and valence Bloch states and envelope functions as well as the optical selection rules are the same as for the SL's,[8] both without and with an applied electric field.

VII. CONCLUSION

We have determined the exact symmetries of conduction and valence-electron states in the [001] $(GaAs)_m(AlAs)_n$ SL's and derived the optical selection rules.

We have also established the approximate symmetry properties of SL's with not too thin slabs of constituent materials. To establish how optical selection rules based on exact Bloch functions correspond to those based on the SL envelope functions, we have approximated the exact symmetry of the SL's with not too thin slabs by a structure with the point symmetry D_{4h} that reflects the SL's structure within the EFA model. We have obtained the approximate Bloch functions and shown that the conduction states form two independent sets having a one-to-one correspondence with the exact conduction states in the D_{2d} group and obeying the same selection rules. We assigned these sets to states originating from Γ electrons of GaAs and X electrons of AlAs. Comparing the selection rules for approximate Bloch states and those rules obtained from experiment, we have established the approximate parities of the Bloch states with respect to inversion and with respect to the change of z to $-z$. In particular, we have shown that electron states in the conduction band always have even or odd parity with respect to the change of z to $-z$, whereas the Γ_5 hole states have both odd and even components. The effects of the spin-orbit interaction have been considered. The application of an electric field parallel to the growth axis induces changes in Bloch-state and envelope-function symmetries. The optical selection rules are then dramatically modified in the z polarization. We have presented the three-dimensional diperiodic space groups of QW's both without and with an applied electric field and shown that the optical selection rules for QW's do not differ from those for SL's.

*Electronic address: tronc@optique.espci.fr

†Permanent address: A. F. Ioffe Physical-Technical Institute, Politekhnicheskaya 26, 194021 St. Petersburg, Russia.

[1] J. Sapriel, J. C. Michel, J. C. Toledano, R. Vacher, J. Kervarec, and A. Regreny, Phys. Rev. B **28**, 2007 (1983).

[2] Yu. E. Kitaev, A. G. Panfilov, P. Tronc, and R. A. Evarestov, J. Phys.: Condens. Matter **9**, 257 (1997).

[3] C. J. Bradley and A. P. Cracknell, *The Mathematical Theory of Symmetry in Solids* (Clarendon, Oxford, 1972).

[4] S. C. Miller and W. F. Love, *Tables of Irreducible Representations of Space Groups and Co-Representations of Magnetic Space Groups* (Pruett, Boulder, CO, 1967).

[5] Bal K. Agrawal and Savitri Agrawal, Phys. Rev. B **45**, 8321 (1992).

[6] D. Scalbert, J. Cernagora, C. Benoit a la Guillaume, M. Maaref, F. F. Charfi, and R. Planel, Solid State Commun. **70**, 945 (1989).

[7] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructures* (Les Editions de Physique, Les Ulis, France, 1990).

[8] P. Tronc, Yu. E. Kitaev, A. G. Panfilov, M. F. Limonov, G. Wang, and V. P. Smirnov, Phys. Rev. B **61**, 1999 (2000).

[9] P. Voisin, G. Bastard, and M. Voos, Phys. Rev. B **29**, 935 (1984).

[10] V. Fiorentini, F. Bernardini, F. Della Sala, A. Di Carlo, and P. Lugli, Phys. Rev. B **60**, 8849 (1999).

[11] E. A. Wood, Bell Syst. Tech. J. **43**, 541 (1964).

[12] R. Melliti, P. Tronc, J. Depeyrot, E. Mao, and A. Majerfeld, Superlattices Microstruct. **23**, 1037 (1998).

[13] P. Tronc, J. Phys. I (France) **2**, 487 (1992); Phys. Status Solidi B **182**, 383 (1994).

[14] Yu. E. Kitaev, A. G. Panfilov, P. Tronc, and R. A. Evarestov, J. Phys.: Condens. Matter **9**, 277 (1997).

[15] J. Bleuse, G. Bastard, and P. Voisin, Phys. Rev. Lett. **60**, 220 (1988).

[16] E. E. Mendez, F. Agullo-Rueda, and J. M. Hong, Phys. Rev. Lett. **60**, 2426 (1988).