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Superlattice band structure in the envelope-function approximation

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The band structure of GaAs-GaAlAs and InAs-GaSb superlattices is calculated by matching propagating or evanescent envelope functions at the boundary of consecutive layers. For GaAs-GaAlAs materials, the envelope functions are the solutions of an effective Hamiltonian in which both band edges and effective masses are position dependent. The effective-mass jumps modify the boundary conditions which are imposed to the eigenstates of the effective-mass Hamiltonian. In InAs-GaSb superlattices, the dispersion relations, although quite similar to those obtained in GaAs-GaAlAs materials, reflect the genuine symmetry mismatch of InAs (electrons) and GaSb (light-holes) levels. The evolution of the InAs-GaSb band structure with increasing periodicity is calculated and found to be in excellent agreement with previous LCAO results. The dispersion relations of heavy-hole bands are obtained.

I. INTRODUCTION

The superlattices,[1] which are tailor-made semiconductors, have recently attracted considerable attention. These materials, grown by molecular-beam epitaxy, consist of alternating layers of two semiconductors of almost equal lattice constant. So far the GaAs-GaAlAs (Ref. 2) and InAs-GaSb (Refs. 3—5) superlattices have been widely studied but few attempts were made to calculate their band structures. Sai-Halasz *et al.*[6] have used linear combination of atomic orbitals (LCAO) approximation to describe the one-dimensional band structure of InAs-GaSb superlattices. Mukherji and Nag,[7] being concerned with GaAs-GaAlAs structures, have calculated their dispersion relations by matching plane-wave-type solutions and their derivatives at the GaAs-GaAlAs boundaries. An attempt to apply the same plane-wave formalism to InAs-GaSb superlattices was apparently unsuccessful.[8] This led Sai-Halasz *et al.*[8] to propose a one-dimensional model of superlattice band structure in which the periodic parts of host-material Bloch functions were included.

In this paper, we will incorporate the superlattice features into a Kane-type analysis[9] of the conduction and valence levels of host materials. The essential point of our model is to neglect any phenomena if rapidly varying at the atomic scale, and to focus attention on the effective Hamiltonian which governs the slowly varying envelope functions. The boundary conditions fulfilled by these envelope functions will be discussed (Sec. II). We will show that previous analysis[7] had overlooked the effective-mass jumps in GaAs-GaAlAs structures; we will derive the dispersion relations valid in these materials (Sec. III). In InAs-GaSb superlattices, the InAs electron states have to be admixed with GaSb light-hole levels. Electrons and light-hole eigenfunctions are orthogonal in host materials, and some trace of this orthogonality is preserved across the interfaces.[8] In fact, the dispersion relations of InAs-GaSb superlattices cannot be obtained by assuming only that the effective masses of the host materials have opposite signs. The allowance of the symmetry mismatch enables a recovery of proper (and simple) dispersion relations. As an application of our results we calculate the evolution with increasing periodicity of InAs-GaSb superlattice band structures for superlattice wave vectors parallel to the superlattice axis (Sec. IV). The envelope-function results are in excellent agreement with LCAO calculations.[6] The heavy-hole dispersion relations will also be discussed (Sec. V).

II. BOUNDARY CONDITIONS IN THE ENVELOPE-FUNCTION APPROXIMATION

In GaAs-GaAlAs and InAs-GaSb superlattices, the band structures of host materials in the vicinity

of the center of the Brillouin zone are quite similar and are well described by the Kane model.[9] For a given superlattice A-B the wave function in each host material takes the form

$$\psi_{A,B}(\vec{r}) = \sum_j F_j^{A,B}(\vec{r}) u_{j_0}^{A,B}(\vec{r}) , \tag{1}$$

where $F_j(\vec{r})$ are slowly varying envelope functions and u_{j_0} is the periodic part of the Bloch functions at $k = 0$. If, for simplicity (but this is not crucial), we neglect the Γ_7 spin-orbit split-off valence band, the $F_j(\vec{r})$ are the solutions of a 6×6 differential system

$$\sum_{j'} D_{jj'} F_{j'}(\vec{r}) = \lambda F_j(\vec{r}) , \tag{2}$$

where the explicit form of $D_{jj'}$ has been given by Kane and λ is the energy. Equivalently, the eigenvalue problem can be expressed in terms of a nonlinear-in-λ 2×2 Hamiltonian. This Hamiltonian acts on the envelope functions associated with two S-type band-edge Bloch functions [hereafter labeled as (1,2)]. Assuming the Kane matrix element π to be identical in A and B host materials, neglecting the free-election kinetic energy $P^2/2m_0$, and choosing the z axis along the superlattice (SL) axis (i.e., perpendicular to the A,B layers) one finds

$$\begin{bmatrix} \mathscr{H}_{11} & \mathscr{H}_{12} \\ \mathscr{H}_{21} & \mathscr{H}_{22} \end{bmatrix} \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} = \lambda \begin{bmatrix} F_1 \\ F_2 \end{bmatrix} , \tag{3}$$

where

$$\begin{aligned} \mathscr{H}_{11} = \mathscr{H}_{22} &= V_S + \pi^2 P_- \frac{1}{\epsilon_A + \lambda - V_P} P_+ + \frac{\pi^2}{3} P_+ \frac{1}{\epsilon_A + \lambda - V_P} P_- \\ &\quad + \frac{2\pi^2}{3} P_z \frac{1}{\epsilon_A + \lambda - V_P} P_z , \\ \mathscr{H}_{12} = \mathscr{H}_{21}^* &= \frac{\pi^2 \sqrt{2}}{3} \left[P_z \frac{1}{\epsilon_A + \lambda - V_P} P_+ - P_+ \frac{1}{\epsilon_A + \lambda - V_P} P_z \right] , \end{aligned} \tag{4}$$

where $P_\pm = (P_x \pm iP_y)/\sqrt{2}$. The energy origin has been taken at the bottom of the A conduction band, and ϵ_A is the energy gap in the A material. V_S and V_P are the shifts of the S and P levels at the point Γ point when going from A to B host materials.

We recall that Eqs. (3) and (4) are valid in each host material but do not give any information on the potential energy associated with the A-B interfaces. Actually, for infinite A or B layers, the (1,2) coupling disappears, and the eigenenergies of (3) are the well-known Kane dispersion relations. For instance, in material A

$$\frac{2\pi^2}{3} \hbar^2 (k_z^2 + 2k_+ k_-) = \lambda(\lambda + \epsilon_A) .$$

We will assume the interface potential to be strongly localized in the vicinity of the A-B interfaces. Its spatial localization is such that at the scale of variation of the slowly varying envelopes the interfaces reduce to the planes

$$\left.\begin{aligned} z &= nd \\ z &= l_A + nd \end{aligned}\right\} n \text{ relative integers} . \tag{5}$$

Moreover, we will assume the interface potential does not mix but only shifts the S- and P-like states at the band edges. For a perfect interface this seems plausible, since A and B have the same spatial symmetry and the same lattice constants. With these *Ansätze* the only effect of the interface on the *envelope* functions F_1 and F_2 is to make the V_S and V_P appearing in Eqs. (4) depend on z through

$$\begin{aligned} V_{S(P)}(z+d) &= V_{S(P)}(z) , \\ V_{S(P)}(z) &= \begin{cases} 0 & \text{if } 0 \le z \le l_A \\ V_{S(P)} & \text{if } l_A < z < l_A + l_B = d , \end{cases} \end{aligned} \tag{6}$$

where l_A and l_B are the A and B layer thicknesses and d is the SL period. The z dependence, although quite simple, has important consequences. Namely, the (1,2) coupling does not vanish in the SL since $\epsilon_A + \lambda - V_P$ does not commute with P_z. In turn, this coupling influences the boundary conditions which F_1 and F_2 should fulfill at the A-B interfaces.

We will assume the envelope functions F_1,F_2 to be continuous at the interface. To obtain two other boundary conditions, we integrate Eqs. (3) and (4) across an interface. Since the 2×2 Hamiltonian [Eq. (3)] is independent of (x,y), $\vec{k}_\perp = (k_x,k_y)$ is a

good quantum number. As long as $V_S(z)$ and $V_P(z)$ have at most finite jumps and making use of the F_1,F_2 continuity, we obtain

$$\frac{1}{\epsilon_A+\lambda-V_P(z)}(-\sqrt{2}F_1' - ik_+F_2)$$

and (7)

$$\frac{1}{\epsilon_A+\lambda-V_P(z)}(-\sqrt{2}F_2' + ik_-F_1) ,$$

both expressions continuous at the interface, where the prime denotes the derivative with respect to z and $k_\pm=(k_x \pm ik_y)/\sqrt{2}$. Furthermore, the long-range behavior of $F_{1,2}$ is governed by the Bloch theorem,

$$F_{1,2}(z+md)=\exp(iqmd)F_{1,2}(z) , \quad (8)$$

valid for any z and any relative integer m. In Eq. (8) q is the SL wave vector along the SL axis.

III. APPLICATION TO GaAs-GaAlAs SUPERLATTICES

In this specific case, we take GaAs as the A material. Then

$$\epsilon_A+\lambda-V_P(z)=\begin{cases}\epsilon_{\text{GaAs}}+\lambda & \text{in GaAs layers}\\ \epsilon_{\text{GaAlAs}}+\lambda-V_S & \text{in GaAlAs layers} .\end{cases}$$

Since GaAs and GaAlAs are wide-gap materials, we may assume in a first approximation $\lambda \ll \epsilon_{\text{GaAs}}$, and $|\lambda-V_S| \ll \epsilon_{\text{GaAlAs}}$ in the energy range of current interest ($0 \lesssim \lambda \lesssim V_S$). If, moreover, $k_\perp \ll l_A^{-1}, l_B^{-1}$, we may neglect the (1,2) coupling and replace Eq. (7) by

$$\frac{1}{\epsilon_{\text{GaAs}}}\frac{dF_{1,2}^{(A)}}{dz}=\frac{1}{\epsilon_{\text{GaAlAs}}}\frac{dF_{1,2}^{(B)}}{dz} . \quad (9)$$

However, in the two-band Kane model $\epsilon_{\text{GaAs}} \propto m_A$ and $\epsilon_{\text{GaAlAs}} \propto m_B$, and Eq. (9) can be rewritten

$$\frac{1}{m_A}\frac{dF_{1,2}^{(A)}}{dz}=\frac{1}{m_B}\frac{dF_{1,2}^{(B)}}{dz} \quad (10)$$

at the interfaces.[10] This boundary condition has not been used before. Instead, one currently assumes[7] the more familiar dF/dz continuity, which is correct only if there are no effective-mass jumps at the boundaries.

The boundary condition equation (10) can be derived in another way. Suppose *ab initio* we assume that only the GaAs and GaAlAs conduction bands come into play, and equivalently that the bands are parabolic in each host material with effective masses m_A and m_B. Then the correct effective Hamiltonian one should use to describe this situation is[11]

$$\mathcal{H}=\frac{1}{4}\left\{p^2,\frac{1}{m(z)}\right\}+V_S(z) . \quad (11)$$

$V_S(z)$ is the periodically varying conduction-band edge defined in Eq. (6). Note in Eq. (11) the presence of the anticommutator $\{\alpha,\beta\}=\alpha\beta+\beta\alpha$. It is imperatively needed to ensure the Hermiticity of $\mathcal{H}$. Assuming the envelope-function eigenstates of (11) to be continuous at the interface and integrating Eq. (11) across an interface, one immediately recovers the boundary condition (10). Let us finally remark that the $(1/m)(dF/dz)$ continuity is the only boundary condition if the continuity of F is given, which ensures the continuity of the probability current, i.e., which guarantees that the eigenstates are stationary. Taking F to be linear combinations of plane waves with opposite wave vectors inside each host material, and using the boundary conditions equations (8) and (10), one readily finds the dispersion relations $\lambda(q)$ in GaAs-GaAlAs superlattices:

$$\cos qd=\cos k_Al_A\cos k_Bl_B-\frac{1}{2}\left[x+\frac{1}{x}\right]\sin k_Al_A\sin k_Bl_B , \quad (12)$$

$$k_A^2=\frac{2m_A}{\hbar^2}\lambda-k_\perp^2 ,$$
$$k_B^2=\frac{2m_B}{\hbar^2}(\lambda-V_S)-k_\perp^2 , \quad (13)$$

$$x=\frac{m_Ak_B}{m_Bk_A} . \quad (14)$$

Let us again stress the fact that Eq. (12) is not identical to the usual Kronig-Penney result, since x explicitly depends on m_A and m_B. Note also that any rapidly varying term like the value of the periodic part of the Bloch function at the interface has disappeared from the final result, Eq. (12). This is coherent with the identification of interfaces with planes. The latter is possible only for functions which vary slowly at the scale of interface.

IV. DISPERSION RELATIONS IN InAs-GaSb SUPERLATTICES

At first sight, it would be very tempting to extend Eq. (12)–(14) to the case of InAs-GaSb superlattices by neglecting in a first approximation the band nonparabolicity. In fact, since $m_A > 0$ and $m_B < 0$, the $1/m(z)][dF/dz)$ continuity leads to a superlattice band structure which shows several similarities but also noticeable differences with the LCAO results.[6] The salient feature of the InAs-GaSb system, when compared with GaAs-GaAlAs material, is the symmetry mismatch between the states of each host material which have to be admixed in the superlattice state: The conduction states of InAs are predominantly *S*-like, whereas light-hole GaSb levels are predominantly *P*-like. It was stressed by Sai-Halasz *et al.*[8] that the symmetry mismatch is preserved across the interfaces (this is in fact one of our basic assumptions), and the building of superlattice states is possible only because of *P* admixture in the InAs electron states and of *S* admixture in the GaSb light-hole levels. The more general Eqs. (7) and (8) should then be used to calculate the dispersion relations. Taking the energy zero at the bottom of the InAs conduction band, we have[15]

$$\left.\begin{aligned} V_P &= \Delta + \epsilon_{\mathrm{InAs}} = 0.56\ \mathrm{eV} \\ V_S &= \Delta + \epsilon_{\mathrm{GaSb}} = 0.96\ \mathrm{eV} \end{aligned}\right\} \text{ if } z \text{ corresponds to a GaSb layer} \tag{15}$$

$V_S = V_P = 0$ if z corresponds to an InAs layer .

Let us assume for simplicity $\vec{k}_\perp = 0$. Then the (1,2) mixing disappears. The superlattice states originating from the matching of InAs conduction states with GaSb light-hole levels have dispersion relations which are still given by Eq. (12). However, in this equation one should replace Eqs. (13) and (14) by

$$\frac{2\pi^2}{3} k_A^2 = \lambda(\lambda + \epsilon_{\mathrm{InAs}}) , \tag{16}$$

$$\frac{2\pi^2}{3} k_B^2 = (\lambda - \Delta)(\lambda - \Delta - \epsilon_{\mathrm{GaSb}}) , \tag{17}$$

$$x = \frac{k_A}{k_B} \frac{\lambda - \Delta}{\lambda + \epsilon_{\mathrm{InAs}}} . \tag{18}$$

In the parabolic limit, x does not reduce to Eq. (14). Instead, for $\lambda << \epsilon_{\mathrm{InAs}}$, one obtains

$$x \approx x_{\mathrm{parabolic}} = \frac{k_A}{k_B} \frac{m_B}{m_A} \frac{\Delta - \lambda}{\epsilon_{\mathrm{GaSb}}} . \tag{19}$$

Note that in Eq. (19) m_B is negative. We see that $x_{\mathrm{parabolic}}$ is equal to the previous result [Eq. (14)] weighted by the ratio of the light-hole kinetic energy to the GaSb band gap, i.e., by a factor which roughly measures the amount of *S*-like level into the predominantly *P*-like GaSb light-hole band.

Assuming $l_A = l_B = d/2$, we have calculated, according to Eqs. (12) and (16)–(18), the evolution with increasing periodicity d of the SL band structure, which arises from the mixing of InAs electron states with GaSb light-hole levels. The results are shown in Fig. 1. Comparing these results with those of LCAO,[6] we see that an almost quantitative agreement is reached between the two models, even in small details such as the anticrossing behavior which takes place near $d \sim 230$ Å (Ref. 5) (and for larger d). We will not discuss further the physical properties implied by the results shown in Fig. 1, since this has been very accurately done by several authors.[3–6]

V. HEAVY-HOLE SUPERLATTICE STATES

Equations (12) and (16)–(18) do not apply to the SL bands which originate from the heavy-hole bands of the host materials. This arises from the fact that

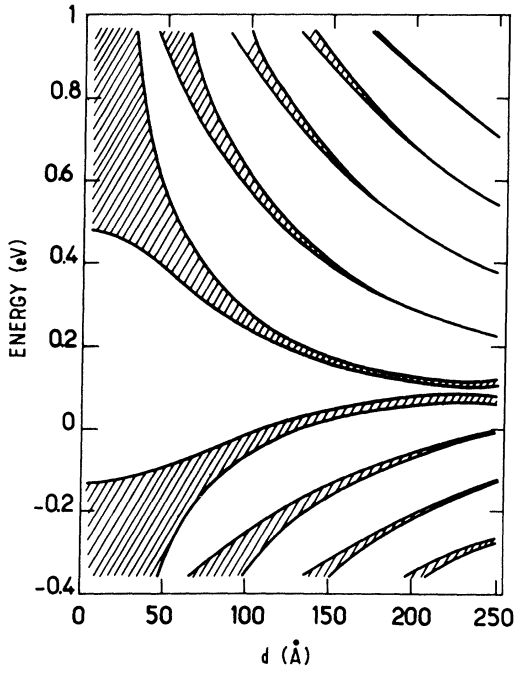

FIG. 1. Calculated subband energies and bandwidths for electrons and light holes as a function of period, assuming $l_A = l_B$ for InAs-GaSb superlattices.

heavy-hole states correspond to vanishing $F_{1,2}$ envelope functions, i.e., the heavy-hole curvature is governed by remote bands not included in the simplified Kane model used throughout this paper.

Still, one may accurately calculate the heavy-hole superlattice bands if $\vec{k}_\perp = 0$. The effect of remote bands in each host material can be incorporated up to order k^2 in the 4×4 matrix acting on the F_i, $i = 3-6$ envelope functions. If $\vec{k}_\perp = 0$, the modified 4×4 matrix is diagonal and the heavy-hole states correspond to $J = \frac{3}{2}$, $m_J = \pm\frac{3}{2}$, i.e., they are entirely decoupled from light-hole states $m_J = \pm\frac{1}{2}$. The $m_J = \pm\frac{3}{2}$ modified matrix elements are simply

$$D_{3/2\pm3/2} = -P_z^2/2M_{A,B} \quad , \tag{20}$$

where $M_{A,B}$ are the heavy-hole effective masses in materials A and B. Owing to the complete decoupling between heavy holes on the one hand and electrons or light holes on the other hand, we see that the heavy-hole SL bands can be calculated exactly in the same way as SL conduction states in "parabolic" GaAs-GaAlAs materials [Eqs. (11)—(14)]. In the InAs-GaSb system, the GaSb layers are potential wells for heavy holes. Measuring the energy from the top of the GaSb (B material here) valence band, and denoting by λ_{hh} the heavy-hole energy, the dispersion relations $\lambda_{hh}(q)$ are given by

$$\cos qd = \cos k_A l_A \cos k_B l_B - \frac{1}{2}\left[x + \frac{1}{x}\right]\sin k_A l_A \sin k_B l_B \quad , \tag{21}$$

$$k_A = \left[\frac{2M_A}{\hbar^2}(\lambda_{hh} - V_{hh})\right]^{1/2} ,$$
$$k_B = \left[\frac{2M_B}{\hbar^2}\lambda_{hh}\right]^{1/2} , \tag{22}$$

where $M_A = 0.4m_0$, $M_B = 0.33m_0$, and $V_{hh} = 0.56$ eV. Since V_{hh} is quite large, the SL heavy-hole bands are almost dispersionless, except for small ($l_A < 20$ Å) InAs thicknesses. Numerical calculations performed for $l_A = l_B$ indicate that the ground heavy-hole band behaves like the ground bound level of a particle confined in a quantum well of infinite depth if $l_B > 150$ Å.

VI. CONCLUSION

We believe the advantage of the envelope-function formalism lies in the simplicity of the final results, Eqs. (12) and (16)—(18), as well as in their generality. For the first time both kinds of existing superlattices are described by the same formalism and the differences in their band structures are naturally explained. Finally, the envelope-function approximation is able to incorporate finite $\vec{k}_\perp$. This will permit a discussion of the transverse motion (i.e., in the layer plane), which is in fact most frequently involved in the experiments.[12—14]

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[1]L. Esaki and R. Tsu, IBM J. Res. Dev. 14, 61 (1970).
[2]R. Dingle, in *Festkorperprobleme* (Advances in Solid State Physics), edited by M. J. Queisser (Pergamon-Vieweg, Braunschweig, 1975), Vol. XV, p. 21.
[3]G. A. Sai-Halasz, in *Proceedings of the 14th International Conference on the Physics of Semiconductors, Edinburgh, 1978,* edited by B. L. H. Wilson (Institute of Physics, London, 1978), p. 21.
[4]L. Esaki, in *Narrow Gap Semiconductors. Physics and Applications,* Vol. 133 of *Lecture Notes in Physics,* edited by W. Zawadzki (Springer, Berlin, 1980), p. 302.
[5]L. L. Chang, in Proceedings of the 15th International Conference on the Physics of Semiconductors, Kyoto, 1980, edited by Shoji Tanaka and Yutaka Toyozawa [J. Phys. Soc. Jpn. 49, Suppl. A, 997 (1980)].
[6]G. A. Sai-Halasz, L. Esaki, and W. A. Harrison, Phys. Rev. B 18, 2812 (1978).
[7]D. Mukherji and B. R. Nag, Phys. Rev. B 12, 4338 (1975).
[8]G. A. Sai-Halasz, R. Tsu, and L. Esaki, Appl. Phys. Lett. 30, 651 (1977).
[9]E. O. Kane, J. Phys. Chem. Solids 1, 249 (1957).
[10]The introduction of a finite spin-orbit coupling does not alter Eq. (10). One should only use the appropriate definition of m_A and m_B in terms of ϵ_A and ϵ_B and the spin-orbit couplings of the host materials.
[11]G. Bastard, J. K. Furdyna, and J. Mycielski, Phys. Rev. B 12, 4356 (1975).
[12]L. Esaki and L. L. Chang, J. Magn. Magn. Mater., 11, 208 (1979).
[13]H. Bluyssen, J. C. Maan, P. Wyder, L. L. Chang, and L. Esaki. Solid State Commun. 31, 75 (1979).
[14]Y. Guldner, J. P. Vieren, P. Voisin, M. Voos, L. L. Chang, and L. Esaki, Phys. Rev. Lett. 45, 1719 (1980).
[15]We take the overlap Δ between the GaSb value band and the InAs conduction band equal to 0.15 eV (Refs. 3—6).