Electric-Field-Induced Localization and Oscillatory Electro-optical Properties of Semiconductor Superlattices

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We show that the application of an electric field F along the growth axis of a semiconductor superlattice results in a strong localization of the eigenstates, a blue shift of the optical-absorption edge, and the presence of oscillations periodic in F^{-1} . These unique electro-optical properties are derived here within the framework of a tight-binding description of the envelope functions and also from numerical solutions of the Schrödinger equation for a finite set of coupled quantum wells.

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In a bulk semiconductor, which usually presents conduction- or valence-band widths $\Delta E_{c,v}$ of a few electronvolts, the application of an electric field F results in the well-known Franz-Keldysh effect¹: The envelope eigenfunctions become Airy functions instead of plane waves, while the optical-absorption coefficient exhibits a low-energy tail below the band gap and an oscillatory behavior above it, characterized by an $F^{-2/3}$ dependence. Conversely, a quantum-well heterostructure displays discrete energy levels ($\Delta E_{c,v} = 0$) and the application of an electric field produces the "quantum-confined Stark effect."^{2,3} A red shift of the optical-absorption edge is observed, as the quantum confinement energies of the ground conduction and valence states E_1 and H_1 are lowered when the potential well is deformed by the electrostatic potential.

Semiconductor superlattices (SL) are unique systems where the bandwidths $\Delta E_{c,v}$ for the carrier motion along the growth axis can be tailored in the range of a few tens of millielectronvolts, while the superperiod *d* falls in the range of a few nanometers. In such systems, electric fields *F* such that $eFd \approx \Delta E_{c,v}$ can easily be applied. This remarkable situation can be approached on an intuitive basis in the following way: The superlattice is a series of quantum wells coupled by the resonant tunnel effect. The tunnel coupling results in the broadening of the energy levels into subbands of widths $\Delta E_{1,}\Delta H_{1}$. The SL band gap is smaller than that of the isolated quantum well by $\frac{1}{2} (\Delta E_1 + \Delta H_1)$. When an electric field is applied along the growth axis, the resonance condition is turned off, as the genuine energy levels in the consecutive quantum wells become misaligned by eFd. The tunnel probability should hence decrease drastically, which in turn means that the eigenstates tend to localize over a few adjacent quantum wells. Then, it can be predicted that the absorption coefficient should tend towards the step function corresponding to a series of uncoupled quantum wells, thus showing a blue shift of the absorption edge of the order of $0.5(\Delta E_1 + \Delta H_1)$.

In this Letter, we demonstrate the relevance of these intuitive and novel statements by studying analytically the electroabsorption in a superlattice within the framework of a tight-binding analysis of the envelope functions.^{4,5} This method contains several approximations, the correctness of which we have checked by solving the problem numerically in the case of a finite set of coupled quantum wells. The later approach closely confirms the validity of the simplified tight-binding treatment, and contradicts recently reported results.⁶

We consider here a (2N+1)-period SL, clad between infinite potential barriers. A constant electric field F is applied along the growth axis z, and the associated electrostatic potential eFz vanishes at the center of the structure. Let $\phi(z)$ be the envelope eigenfunction of the ground state of an isolated quantum well centered at the origin. In the simple nearest-neighbor tight-binding analysis, we retain only one level per quantum well, and the SL eigenstates are expanded as

$$\chi_q(z) = \sum_{-N}^{+N} c_{nq} \phi(z - nd). \tag{1}$$

At zero electric field, this method leads to the wellknown quasicontinuous spectrum of the conduction miniband:

$$\epsilon_q = E_1 - 2\lambda_c \cos(qd), \text{ with } qd = i\pi/2(N+1) \quad (1 \le i \le 2N+1), \tag{2}$$

where λ_c is the modulus of the transfer integral between nearest neighbors. The corresponding eigenfunctions are extended through the entire structure, as

$$c_{nq} = [1/(N+1)]^{1/2} \begin{cases} \sin(nqd), & \text{with } qd = j\pi/(N+1) \quad (1 \le j \le N), \\ \cos(nqd), & \text{with } qd = (j' + \frac{1}{2})\pi/(N+1) \quad (0 \le j' \le N). \end{cases}$$
(3)

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With the same assumptions, in presence of an electric field F strong enough so that the total potential drop is larger than the miniband width $(NeFd \gg 2\lambda_c)$, the same tight-binding analysis predicts that the miniband spectrum [Eq. (2)] is replaced by an evenly spaced spectrum hereafter called a Wannier-Stark ladder,

$$\epsilon_v = E_1 + veFd, \quad -N \le v \le +N, \tag{4}$$

and the corresponding eigenfunctions are given by Eq. (1), with

$$c_{nv} = J_{n-v}(2\lambda_c/eFd), \qquad (5)$$

where J_m is the Bessel function of integer index *m*. The asymptotic expansion of $J_{n-\nu}$ for small arguments yields

$$c_{nv} \approx [1/(|n-v|)!] (\lambda_c/eFd)^{|n-v|},$$
 (6)

which corresponds, at large electric field, to a faster than

exponential localization of the wave function of state v in the vicinity of the quantum well of the same index, a result already quoted in the literature.^{5,7}

It can be shown by various means that the difference between the exact spectrum and the regularly spaced ladder [Eq. (4)] is an edge effect, which becomes negligible for most of the states v < N, as soon as N becomes large. For example, for a 51-period 30-Å-50-Å GaAs- $Al_{0.3}Ga_{0.7}As$ SL, 49 conduction states obey Eq. (4) to a very good approximation at an electric field of 5 kV/cm. Hence it is relevant to calculate the optical absorption of a SL with use of the spectrum given by Eq. (4) and the related wave functions [Eq. (5)], and analogous formulas for the hole states. We consider a type-I SL, in which the electrons and the holes are confined in the same layers (e.g., GaAs-AlGaAs), and we assume parabolic inplane dispersion relations for both particles. In the limit of thick superlattices, the absorption is found to be equal to

$$\alpha(\hbar\omega) = (2N+1)\alpha_0 \sum_{m=-N}^{+N} J_m^2 (-2/f) Y(\hbar\omega - (E_g + E_1 + H_1 + meFd)),$$
(7)

where E_g is the band gap of the well material, Y is the unit step function, and $f = eFd/(\lambda_c + \lambda_v)$. The prefactor α_0 is equal to $2\pi e^2 P^2 M/ncm_0^2 \hbar^2 \omega \approx 0.006$ where M is the in-plane reduced mass of the electron-hole pair, P is the Kane matrix element, and n is the optical index.⁴

The evolution of the absorption spectrum of a 41period SL with increasing values of f is shown in Fig. 1. The absorption for a rather small value of the reduced electric field f=0.2 is close to the zero-field absorption, which shows the relevance of the Wannier-Stark spectrum even at such a small field. On the other hand, for f=4, which corresponds to a voltage drop between adja-



FIG. 1. Absorption of a 41-period superlattice, normalized to $(2N+1)\alpha_0$, vs the reduced photon energy $\epsilon = [h\omega - (E_g + E_1 + H_1)]/(\lambda_c + \lambda_v)$, for increasing values of the reduced electric field $f = eFd/(\lambda_c + \lambda_v)$.

cent wells equal to the sum of the zero-field conductionand valence-band widths, the absorption coefficient is indeed close to the step function at $E_{g} + E_{1} + H_{1}$ which we would obtain for a series of uncoupled quantum wells. Although the region of allowed absorption is wider at f=4 than at f=0 and in particular not strictly vanishing below the SL bandgap, the absorption edge at f=4is effectively shifted to the blue with respect to the f=0one. In fact, at this field, the other steps at lower and higher energy accommodate only 10% of the total absorption. These steps, which occur at energies $(E_g + E_1)$ $+H_1$)+peFd (p = ± 1, ± 2, ...), correspond to oblique transitions in real space, connecting the nth conductionband state (localized near the nth well) with the (n+p)th valence state, localized in the (n+p)th quantum well. Note that this effective blue shift is much larger than the well-known red Stark shift which would be observed in the equivalent isolated quantum well. Indeed, with the parameters of the GaAs-Ga_{0.7}Al_{0.3}As system, well and barrier thicknesses of 35 Å are required to obtain a 45-meV conduction-band width. The condition f = 4 (see Fig. 1) then corresponds to a field of 65 kV/cm. At this field, the Stark shift in a 35-Å-thick quantum well² is smaller than 1 meV, to be compared to a 22-meV blue shift.

The absorption coefficient at a fixed energy inside the F=0 miniband oscillates with the electric field. These oscillations, which are periodic in F^{-1} , are distinct from the Franz-Keldysh oscillations. This F^{-1} periodicity, illustrated in Fig. 2(a), is strongly reminiscent of the Shubnikov-de Haas effect. Indeed, in both cases, one deals with an evenly spaced spectrum (Landau levels or a Wannier-Stark ladder) which, by a sweeping of the



FIG. 2. (a) f^{-1} oscillations of the absorption at a fixed reduced photon energy close to the SL band gap, calculated for a 201-period SL. (b) Convergence of the SL absorption toward the Franz-Keldysh oscillations, calculated for a 4001-period SL and a very small reduced electric field $f = 1.5 \times 10^{-3}$.

external field (B or F), is made to cross a fixed energy (the Fermi energy or the excess photon energy with respect to $E_g + E_1 + H_1$). However, as shown in Fig. 2(b), these new oscillations give way to the Franz-Keldysh effect when the calculation is made for "bulklike" conditions, i.e., a small enough $F(f \ll 1)$, a thick enough SL ($Nf \gg 1$), and a photon energy close enough to the SL band gap. In fact, this limiting behavior can be derived analytically from Eq. (7) by use of the Langer asymptotic expansions of the Bessel functions.⁸

Finally, an important feature seen in Fig. 1 is that the absorption always saturates at the same value $(2N + 1)\alpha_0$, which results from the Graf sum rule on the Bessel functions in Eq. (7). This is in contradiction with the results reported in Ref. 6.

The tight-binding approach described above has the advantage of simplicity, but it is not fully justified since we have neglected the coupling of the Wannier-Stark states originating from the fundamental quantum-well bound state with all the other (bound or unbound) states of the wells located in the lower potential region. To check the accuracy of this approach, we have numerically solved the Schrödinger equation for the envelope functions in the structure sketched in Fig. 3(a). The structure consists of N coupled quantum wells embedded between thick barriers, themselves terminated by infinite potential barriers at both ends. The electric potential is approximated by a piecewise-constant potential, as



FIG. 3. Sketch of the heterostructure considered in the numerical approach, (a) at zero electric field and (b) in a discretized potential simulating an electric field of 30 kV/cm. Also shown is the square of the modulus of the eigenfunction corresponding to a state near the center of the miniband. Calculations are made with use of the band parameters of the GaAs-Al_{0.3}Ga_{0.7}As system, and well and barrier thicknesses of 35 Å.

shown in Fig. 3(b). With this approximation, the eigenfunction in each layer is the sum of an incoming and a reflected plane wave (instead of Airy functions), connected at each interface by means of the well-known rules of the envelope-function formalism. This treatment allows us to take into account nonparabolicity, which can be an important ingredient of the bandwidth in a real system, and is particularly convenient from the computational point of view. In Figs. 3(a) and 3(b) we have also displayed the square of the modulus of the wave function of a representative extended state near the center of the conduction miniband, and its rapid localization over three adjacent quantum wells in a moderate electric field of 30 kV/cm.

Though of course limited to systems with a relatively small number of layers, the numerical approach closely confirms the results of the tight-binding analysis. For example, the absorption obtained for a six-well structure is essentially identical to that of Fig. 1. In particular, the saturation of the absorption at $(2N+1)\alpha_0$ is very weakly (less than 3%) affected by the presence of a number of states energetically located above the barrier in the region of low electrostatic potential [Fig. 3(b)], which simulate the continuum that would be present in a thick superlattice. This shows that the localized Wannier-Stark states are weakly coupled to the continuum, which in turn justifies the tight-binding approach.

The localization of the wave functions will also exist for a type-II superlattice where the conduction- and valence-band wave functions are concentrated in adjacent layers. In this case, an electron localized in a given layer will be optically coupled to two hole states, localized in the adjacent layers, and thus having different energies. In this case, we expect that in the high-field limit, the absorption tends toward a double step at E_g $+E_1+H_1\pm 0.5eFd$. This result is also obtained analytically with the tight-binding method.

In conclusion, we have shown that unique electrooptical effects should exist in semiconductor superlattices. These new effects are characterized by a strong field-induced localization of the eigenstates, a blue shift of the optical-absorption edge, and oscillations of the absorption coefficient periodic in F^{-1} . Besides its obvious potential usefulness to the design of new electro-optical modulators, this localization effect should lead to many rather unexpected consequences such as a field-induced enhancement of the exciton binding energy from a 3D to a 2D regime if the bandwidth is larger than the 3D Rydberg energy. The present effect is also a key to a quantum study of the transport properties of superlattices at large electric fields applied along the growth axis.

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