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Resonant states in $GaAs/Ga_{1-x}Al_xAs$ quantum wells: theoretical analysis of the density of states and phase times

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Abstract. The existence of sharp resonant states in a single quantum well separated from its semi-infinite substrate by a barrier layer is reported here. These resonances appear as well defined peaks in the density of states. The local and total densities of states are obtained from an analytical determination of the Green functions. The expressions of the transmission and reflection phase times are also derived and compared to the density of states. The positions of the peaks in the density of states enable us to study the energy levels of resonant states as a function of the thicknesses of the barrier and well layers. Specific applications of our analytical results are given in this paper for a $GaAs/Ga_{0.7}Al_{0.3}As$ bilayer sandwiched between two semi-infinite GaAs and $Ga_{0.7}Al_{0.3}As$ media.

1. Introduction

A great deal of work has been devoted during the last decade to the study of electron states confined inside a spatial zone, often called a 'well', of finite size along at least one direction. In such systems, the medium surrounding the well must form a 'barrier' which prevents the well wave function from extending much outside it. In particular, it has been shown recently [1–4] that the ideal quantum well (QW) potential in which one considers a QW system to be terminated on either side by barriers of finite height, but infinite in extent, needs to be modified to take into account the finite-size effect of the barriers surrounding the QW. Moison *et al* [1] have performed an extended study by *in situ* photoluminescence on the effect of a cap layer (barrier of finite extent) on bound states in $GaAs/Ga_{0.7}Al_{0.3}As$ QWs and their interaction with surface states. Fafard *et al* [2, 3] have studied the effect of the high potential at the device surface on the above barrier (continuum) states in a simple $GaAs/In_xGa_{1-x}As$ structure; intense above-barrier oscillations related to the oscillations in the probabilities of finding carriers in the various region induced by finite cap layers were observed in photoluminescence spectra. Above-barrier optical transitions in $Ga_{1-x_1}Al_{x_1}As/GaAs/Ga_{1-x_3}Al_{x_3}As$ compositionally asymmetric single QWs have also been investigated with piezomodulation spectroscopy by Parks *et al* [4]; in particular they have observed the presence of quasibound resonant states existing in the continuum between the barrier energies in both the conduction and the valence bands. However, in all these studies the effect of the substrate (i.e., a buffer layer of large extent), which serves as support for the devices, on electron states in these structures is usually ignored, except in [5] where the substrate affects only continuum states situated above the barriers of the well.

In this paper, we examine below- and above-barrier resonant states in a single GaAs QW of thickness d_2 (see figure 1) confined on one side by a $Ga_{0.7}Al_{0.3}As$ barrier of infinite extent and on the other side by a $Ga_{0.7}Al_{0.3}As$ barrier of finite extent (cap layer of thickness d_1). The whole system is deposited on a GaAs substrate which represents the buffer layer of infinite extent. Among different mathematical approaches, the Green function method is quite suitable for studying the spectral properties of these composite materials; in particular, it enables us to calculate the total or local density of states (DOS) in which the resonant states appear as well defined peaks. The Green function approach allowed us also to determine the transmission and reflection rates as well as the phase times. The phase times are considered [6] to be relevant physical times to describe the motion of wave packets narrow in wave-number space. There are several other times [7–9]; however the only well defined and well established one [8] is the 'dwell time' which is the average time spent in a given region by all incoming particles. We show that the positions of the resonances obtained from DOS coincide with those given by phase times and transmission rates. The halfwidth of the peaks in the DOS and phase times are related to the lifetime of the resonant states. The Green function used here is calculated by using the interface response theory in composite materials [10] in which the solution is first searched in the restricted space of interfaces before being extended to the whole material (see below).

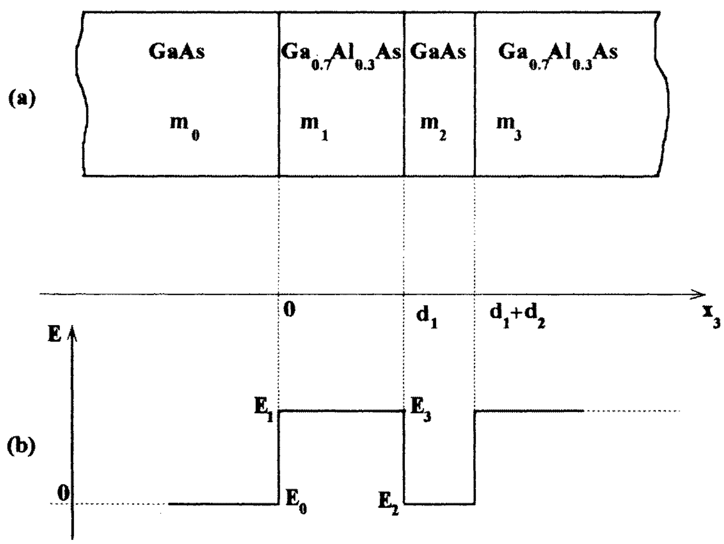

Figure 1. Schematic representation (a) and potential profile (b) of a single quantum well with a well layer GaAs surrounded by two $Ga_{0.7}Al_{0.3}As$ barriers of finite and infinite extent; the whole system is deposited on a GaAs substrate. d_1 and d_2 are respectively the thickness of the barrier and well layers.

The organization of this paper is as follows: section 2 presents the analytical results for the Green functions and densities of states. Section 3 gives the expressions of the transmission and reflection rates. Section 4 shows the numerical results for the structure depicted in figure 1.

2. Density of states calculation

2.1. The Green function calculation

An approximate and simple expression of the change in the density of states (DOS) $\Delta n(E)$ is given by Trzeciakowski *et al* [11] for single- and double-barrier structures. The local DOS is also analysed in the same structure by Bahder *et al* [12]. These DOSs are obtained by calculating the eigenfunctions of an effective-mass Schrödinger equation. In this section, we give an exact and complete calculation of local and total DOS associated with the structure depicted in figure 1. We calculate the DOS by using the theory of interface response in composite material [10]. In this theory, the Green function $\mathbf{g}$ of a composite system can be written as [10]

$$\mathbf{g}(DD) = \mathbf{G}(DD) + \mathbf{G}(DM)\mathbf{G}^{-1}(MM)[\mathbf{g}(MM) - \mathbf{G}(MM)]\mathbf{G}^{-1}(MM)\mathbf{G}(MD) \tag{1}$$

where D and M are respectively the whole space and the space of the interfaces in the composite material. In the continuum model, M is just limited to the planes $x_3 = 0$, d_1 and $d = d_1 + d_2$ (see figure 1). $\mathbf{G}$ is a block-diagonal matrix in which each block $\mathbf{G}_i$ corresponds to the bulk Green function of the subsystem i. In our case, the composite material is composed of slabs of materials i ($i = 1, 2$) with thickness d_i sandwiched between two semi-infinite materials $i = 0$ and $i = 3$. In equation (1), the calculation of $\mathbf{g}(DD)$ requires, besides $\mathbf{G}_i$, the knowledge of $\mathbf{g}(MM)$. In practice, the latter is obtained by inverting the matrix $\mathbf{g}^{-1}(MM)$ which can be simply built from a juxtaposition of the matrix $\mathbf{g}_{si}^{-1}(MM)$, where $\mathbf{g}_{si}(MM)$ is the interface Green function of the slab i ($i = 1, 2$) and of the substrate j ($j = 0, 3$) alone [10] with stress-free boundary conditions.

Therefore the first step before addressing the problem of layered materials will be to know the surface element of the Green function $\mathbf{g}_{si}$ of a slab of medium i and substrate j with stress-free boundary conditions. These surface elements can be written [10] in the case of a slab as a (2×2) matrix $\mathbf{g}_{si}(M_i M_i)$, within the interface space M_i, namely

$$\mathbf{g}_{si}^{-1}(M_i M_i) = \begin{bmatrix} A_i & B_i \\ B_i & A_i \end{bmatrix} \tag{2}$$

where

$$M_i \equiv \{0, d\} \text{ for } i = 1 \text{ and } M_i \equiv \{d_1, d = d_1 + d_2\} \text{ for } i = 2$$

$$A_i = -F_i \frac{C_i}{S_i} \qquad B_i = \frac{C_i}{S_i} \qquad C_i = \cosh \alpha_i d_i \qquad S_i = \sinh \alpha_i d_i \tag{3}$$

$$F_i = \frac{\hbar^2}{2m_i}\alpha_i \qquad \alpha_i^2 = -\frac{2m_i}{\hbar^2}(E - E_i) \text{ with } i = 1, 2$$

while in the case of the substrate j, the surface element is given by [10]

$$\mathbf{g}_{sj}^{-1}(M_j M_j) = -F_j \qquad (j = 0, 3) \tag{4}$$

where

$$M_j \equiv \{0\} \text{ for } j = 0 \text{ and } M_j \equiv \{d\} \text{ for } j = 3.$$

Thus, the inverse of the Green function within the total interface space M is obtained by a juxtaposition of the matrices $\mathbf{g}_{si}^{-1}(M_i M_i)$ (2) and $\mathbf{g}_{si}^{-1}(M_j M_j)$ (4) (see equation (2.43c) of [10])

$$\mathbf{g}^{-1}(MM) = \begin{bmatrix} -F_0 - \frac{F_1 C_1}{S_1} & \frac{F_1}{S_1} & 0 \\ \frac{F_1}{S_1} & -\frac{F_1 C_1}{S_1} - \frac{F_2 C_2}{S_2} & \frac{F_2}{S_2} \\ 0 & \frac{F_2}{S_2} & -\frac{F_2 C_2}{S_2} - F_3 \end{bmatrix} \tag{5}$$

where $M \equiv \{0, d_1, d\}$. By inverting the matrix $\mathbf{g}^{-1}(MM)$, we obtain

$$\mathbf{g}(MM) = -\frac{1}{W}\begin{bmatrix} C_1C_2 + \frac{F_2}{F_1}S_1S_2 + \frac{F_3}{F_2}C_1S_2 + \frac{F_3}{F_1}C_2S_1 & C_2 + \frac{F_3}{F_2}S_2 & 1 \\ C_2 + \frac{F_3}{F_2}S_2 & C_1C_2 + \frac{F_0}{F_1}C_2S_1 + \frac{F_3}{F_2}C_1S_2 + \frac{F_0F_3}{F_1F_2}S_1S_2 & C_1 + \frac{F_0}{F_1}S_1 \\ 1 & C_1 + \frac{F_0}{F_1}S_1 & C_1C_2 + \frac{F_0}{F_2}C_1S_2 + \frac{F_0}{F_1}C_2S_1 + \frac{F_1}{F_2}S_1S_2 \end{bmatrix} \tag{6}$$

where

$$W = C_1C_2(F_0 + F_3) + C_1S_2\left(\frac{F_0F_3}{F_2} + F_2\right) + C_2S_1\left(\frac{F_0F_3}{F_1} + F_1\right) + S_1S_2\left(\frac{F_1F_3}{F_2} + \frac{F_0F_2}{F_1}\right). \tag{7}$$

From the knowledge of these interface matrix elements one can obtain the Green function between any two points of the whole system (see (1)). However, as we are interested in the calculation of the DOS, we only give their expressions for two points belonging both either to the two substrates ($j = 0, 3$) or to the two layers ($i = 1, 2$).

Let us recall first that the bulk Green function of the medium i is given by [10]

$$G_i(x_3, x_3') = -\frac{e^{-\alpha_i|x_3 - x_3'|}}{2F_i} \tag{8}$$

where α_i and F_i are given by (3).

Thus, the Green function between any two points of each medium i is given by equations (1), (6) and (8), and can be written as follows:

(i) when the two points are inside the medium $i = 0$ ($x_3, x_3' \leqslant 0$)

$$g(x_3, x_3') = -\frac{e^{-a_0|x_3 - x_3'|}}{2F_0} + \left\{\frac{1}{2F_0} - \frac{1}{W}\left[C_1C_2 + \frac{F_2}{F_1}S_1S_2 + \frac{F_3}{F_2}C_1S_2 + \frac{F_3}{F_1}C_1S_1\right]\right\} e^{\alpha_0(x_3' + x_3)} \tag{9}$$

(ii) when the two points are inside the medium $i = 1$ ($0 \leqslant x_3, x_3' \leqslant d_1$)

$$g(x_3, x_3') = -\frac{e^{-\alpha_1|x_3 - x_3'|}}{2F_1} + \frac{1}{S_1^2}\{A\sinh(\alpha_1(d_1 - x_3))\sinh(\alpha_1(d_1 - x_3')) + B[\sinh(\alpha_1 x_3)\sinh(\alpha_1(d_1 - x_3')) + \sinh(\alpha_1(d_1 - x_3))\sinh(\alpha_1 x_3')] + C(\sinh(\alpha_1 x_3)\sinh(\alpha_1 x_3'))\} \tag{10}$$

where

$$A = -\frac{1}{W}\left(C_1C_2 + \frac{F_2}{F_1}S_1S_2 + \frac{F_3}{F_2}C_1S_2 + \frac{F_3}{F_1}C_2S_1\right) + \frac{1}{2F_1} \tag{11}$$

$$B = -\frac{1}{W}\left(C_2 + \frac{F_3}{F_2}S_3\right) + \frac{e^{-\alpha_1 d_1}}{2F_1} \tag{12}$$

and

$$C = -\frac{1}{W}\left(C_1C_2 + \frac{F_0}{F_1}C_2C_1 + \frac{F_3}{F_2}C_1S_2 + \frac{F_0F_3}{F_1F_2}S_1S_2\right) + \frac{1}{2F_1} \tag{13}$$

(iii) when the two points are inside the medium $i = 2$ ($d_1 \leqslant x_3, x_3' \leqslant d$)

$$\begin{aligned} g(x_3, x_3') = &-\frac{\mathrm{e}^{-\alpha_2|x_3-x_3'|}}{2F_2} + \frac{1}{S_2^2}\{D\sinh(\alpha_2(d-x_3))\sinh(\alpha_2(d-x_3')) \\ &+E[\sinh(\alpha_2(d-x_3))\sinh(\alpha_1(x_3'-d_1)) \\ &+\sinh(\alpha_2(x_3-d_1))\sinh(\alpha_2(d-x_3'))] \\ &+F\sinh(\alpha_2(x_3-d_1))\sinh(\alpha_1(x_3'-d_1))\} \end{aligned} \tag{14}$$

where

$$D = -\frac{1}{W}\left(C_1C_2 + \frac{F_0}{F_1}C_2S_1 + \frac{F_3}{F_2}C_1S_2 + \frac{F_0F_3}{F_1F_2}S_1S_2\right) + \frac{1}{2F_2} \tag{15}$$

$$E = -\frac{1}{W}\left(C_1 + \frac{F_0}{F_1}S_1\right) + \frac{\mathrm{e}^{-\alpha_2 d_2}}{2F_2} \tag{16}$$

$$F = -\frac{1}{W}\left(C_1C_2 + \frac{F_1}{F_2}S_1S_2 + \frac{F_0}{F_1}C_2S_1 + \frac{F_0}{F_2}C_1S_2\right) + \frac{1}{2F_2} \tag{17}$$

(iv) when the two points are inside the medium $i = 3$ ($x_3, x_3' \geqslant d$)

$$\begin{aligned} g(x_3, x_3') = &-\frac{\mathrm{e}^{-\alpha_3|x_3-x_3'|}}{2F_3} \\ &+\left\{\frac{1}{2F_3} - \frac{1}{W}\left[C_1C_2 + \frac{F_1}{F_2}S_1S_2 + \frac{F_0}{F_2}C_1S_2 + \frac{F_0}{F_1}C_2S_1\right]\right\}\mathrm{e}^{-\alpha_3(x_3'+x_3-2d)}. \end{aligned} \tag{18}$$

2.2. *The local density of states*

The local density of state on the plane x_3 is given by

$$n(E, x_3) = -\frac{1}{\pi}\,\mathrm{Im}\,g^+(E, x_3) \tag{19}$$

where

$$g^+(E, x_3) = \lim_{\varepsilon\to 0} g(E + \mathrm{i}\varepsilon, x_3) \tag{20}$$

and $g(E)$ is the above-defined Green's function.

2.3. *The total density of states*

The total density of states is obtained by integrating over x_3 the local density of states in the above-defined composite system (figure 1) from which the contribution of the bulk of the semi-infinite media are subtracted. This variation $\Delta n(E)$ can be written as

$$\Delta n(E) = \Delta n_0(E) + n_1(E) + n_2(E) + \Delta n_3(E) \tag{21}$$

where $\Delta n_0(E)$ and $\Delta n_3(E)$ are the variation of the DOS in media $i = 0$ and $i = 3$ respectively and $n_1(E)$ and $n_2(E)$ the DOS in the layers 1 and 2 respectively. These four quantities are given by

$$\Delta n_0(E) = -\frac{1}{\pi}\mathrm{Im}\int_{-\infty}^{0}[g(x_3, x_3) - G_0(x_3, x_3)]\,\mathrm{d}x_3 \tag{22}$$

$$n_1(E) = -\frac{1}{\pi}\mathrm{Im}\int_{0}^{d_1}[g(x_3, x_3)]\,\mathrm{d}x_3 \tag{23}$$

$$n_2(E) = -\frac{1}{\pi}\mathrm{Im}\int_{d_1}^{d}[g(x_3, x_3)]\,\mathrm{d}x_3 \tag{24}$$

$$\Delta n_3(E) = -\frac{1}{\pi}\mathrm{Im}\int_{d}^{+\infty}[g(x_3, x_3) - G_3(x_3, x_3)]\,\mathrm{d}x_3. \tag{25}$$

g, G_0 and G_3 are, respectively, the Green function of the whole system depicted in figure 1, the substrate (0) and the semi-infinite medium (3). With the help of the explicit expressions of the Green functions given above ((8)–(10), (14), (18) and (22)–(25)), we obtain

$$\Delta n_0(E) = -\frac{1}{\pi}\mathrm{Im}\left\{\frac{1}{2\alpha_0}\left[\frac{1}{2F_0} - \frac{1}{W}\left(C_1C_2 + \frac{F_2}{F_1}S_1S_2 + \frac{F_3}{F_2}C_1S_2 + \frac{F_3}{F_1}C_2S_1\right)\right]\right\} \tag{26}$$

$$n_1(E) = -\frac{1}{\pi}\mathrm{Im}\left(-\frac{d_1}{2F_1} + \frac{1}{2\alpha_1 S_1^2}[(A + C)(C_1S_1 - \alpha_1 d_1) + 2B(\alpha_1 d_1 C_1 - S_1)]\right) \tag{27}$$

$$n_2(E) = -\frac{1}{\pi}\mathrm{Im}\left(-\frac{d_2}{2F_2} + \frac{1}{2\alpha_2 S_2^2}[(D + F)(C_2S_2 - \alpha_2 d_2) + 2E(\alpha_2 d_2 C_2 - S_2)]\right) \tag{28}$$

$$\Delta n_3(E) = -\frac{1}{\pi}\mathrm{Im}\left\{\frac{1}{2\alpha_3}\left[\frac{1}{2F_3} - \frac{1}{W}\left(C_1C_2 + \frac{F_1}{F_2}S_1S_2 + \frac{F_0}{F_2}C_1S_2 + \frac{F_0}{F_1}C_2S_1\right)\right]\right\}. \tag{29}$$

3. Reflected and transmitted waves

The deformation $|\psi(D)\rangle$ of a composite material is given by [10]

$$|\psi(D)\rangle = |\Psi(D)\rangle - \mathbf{G}(DM)\mathbf{G}^{-1}(MM)|\Psi(M)\rangle + \mathbf{G}(DM)\mathbf{G}^{-1}(MM)\mathbf{g}(MM)\mathbf{G}^{-1}(MM)|\Psi(M)\rangle \tag{30}$$

where $|\Psi(D)\rangle$ represents the deformation of the reference system. In particular, if $|\Psi(D)\rangle$ is a wave function of incident electrons in the substrate $i = 0$ represented by the plane wave $\Psi_0(x_3) = \mathrm{e}^{-\alpha_0 x_3}$ of unit amplitude, equation (30) enables us to calculate all the waves reflected and transmitted by the interfaces.

With the help of the Green functions given above ((6) and (8)), the deformation $\psi_0(x_3)$ in the substrate (0) is found to be

$$\psi_0(x_3) = \mathrm{e}^{-\alpha_0 x_3} + \left\{-1 + \frac{2F_0}{w}\left[C_1C_2 + \frac{F_2}{F_1}S_1S_2 + \frac{F_3}{F_2}C_1S_2 + \frac{F_3}{F_1}C_2S_1\right]\right\}\mathrm{e}^{\alpha_0 x_3} \tag{31}$$

while in the semi-infinite medium (3), we obtain

$$\psi_3(x_3) = \mathrm{e}^{-\alpha_3 x_3} - \frac{2F_0}{W}\,\mathrm{e}^{-\alpha_3(x_3 - d)}. \tag{32}$$

The first term in the right-hand side of equations (31) and (32) corresponds to the incident wave function of the electrons, while the second term is associated with the wave function of the reflected and transmitted electrons in the substrate $i = 0$ and in the semi-infinite medium $i = 3$ respectively. These later quantities are expressed, respectively, as

$$C_R\,\mathrm{e}^{\alpha_0 x_3} \text{ and } C_T\,\mathrm{e}^{-\alpha_3(x_3-d)} \tag{33}$$

where

$$C_R = \frac{2F_0}{W}\left(C_1C_2 + \frac{F_2}{F_1}S_1S_2 + \frac{F_3}{F_2}C_1S_2 + \frac{F_3}{F_1}C_2S_1\right) - 1 \tag{34}$$

and

$$C_T = -\frac{2F_0}{W}. \tag{35}$$

C_R and C_T are the reflection and transmission amplitudes respectively. The reflection rate R and transmission rate T are defined by

$$R = |C_R|^2 \text{ and } T = |C_T|^2. \tag{36}$$

The reflection and transmission phase times, i.e. the time that it takes the peak of a wave packet to appear on the left and right sides of the double layers ($i = 1, 2$) are given respectively, in the stationary phase approximation, by [13, 14]

$$\tau_R = \bar{h}\frac{\mathrm{d}\theta_R}{\mathrm{d}E} \text{ and } \tau_T = \bar{h}\frac{\mathrm{d}\theta_T}{\mathrm{d}E} \tag{37}$$

where $h = 2\pi\bar{h}$ is the Planck constant and θ_R and θ_T are the phases of the reflected and transmitted amplitudes of electrons scattered off the two embedded layers.

4. Numerical results

For the numerical calculations, we investigate the existence and behaviour of resonant states (called also leaky waves) in a GaAs well sandwiched between a $Ga_{0.7}Al_{0.3}$As barrier of infinite extent and a $Ga_{0.7}Al_{0.3}$As barrier whose thickness is variable, the whole system is deposited on a GaAs substrate (figure 1). The effective mass of the electron inside the well and barrier are [15] 0.067 m_0 and 0.0919 m_0, respectively, where $m_0 = 9.11 \times 10^{-31}$ kg. The barrier height is [15] 283.2 meV. Even though we are dealing with the system depicted in figure 1, our calculation could be utilized also for a system with different potential configuration.

Figure 2 gives an illustration of the dispersion curves of energy levels in the structure depicted in figure 1. The thickness of the GaAs well is such that $d_2 = 70$ Å and the thickness d_1 of the barrier layer is taken to be variable. All the branches in figure 2 represent resonant states induced by the $Ga_{0.7}Al_{0.3}$As/GaAs bilayer in the continuum of the bulk bands of GaAs substrate and $Ga_{0.7}Al_{0.3}$As barrier of infinite extent. These resonant states are obtained from the maxima of the DOS, shown in figure 3 for a few values of the thickness d_1. The full horizontal line in figure 2 represents the position of the energy level $E_3 = E_1$. The two curves situated below E_3 represent resonant waves of the well, and appear as well defined peaks in the DOS of figure 3, even though they are in resonance with the bulk states of the GaAs substrate, the corresponding energies of these resonances present a very small variation with d_1 (see figure 2). Note that for the sake of illustration of very narrow peaks, the resonances in figure 3 are enlarged by adding a small imaginary part ε to the energy E. Moreover, the intensity of the resonances below E_3 increases by increasing the thickness d_1 of the $Ga_{0.7}Al_{0.3}$As barrier, and for large values of d_1 (see figure 3(d)), the resonances appear as delta functions of weight 1 as the interaction between the GaAs well and the GaAs substrate becomes very weak. Let us mention that

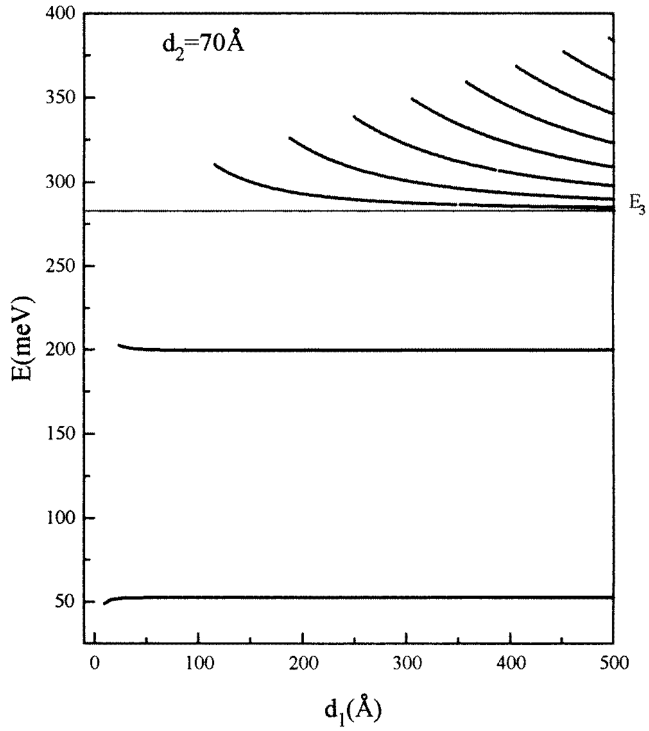

Figure 2. Variation of the energy levels of resonant states, for $d_2 = 70$ Å, as a function of d_1 where d_1 and d_2 are respectively the thickness of the $Ga_{0.7}Al_{0.3}As$ barrier and GaAs well. The horizontal full line indicates the position of the barrier height E_3.

similar results are found by Moison *et al* [1], where the energy position and intensity of the photoluminescence originating from the GaAs well are attributed to the coupling of GaAs confined states with surface states confined in a very thin GaAs well located at the surface of the device. On the other hand, we obtain the same behaviour as in figure 3 for the DOS (not given here) on changing the height of the barrier layer, namely the intensity of resonances increases on increasing the height of the barrier layer, while the height of the barrier of infinite extent (figure 1) is kept constant. Concerning the curves lying above E_3 in figure 2, they present a noticeable variation with varying d_1 and tend asymptotically to the limit of E_3 when $d_1 \to \infty$. These resonances correspond to waves with predominant amplitudes in the $Ga_{0.7}Al_{0.3}As$ barrier (see below), even though they are propagating in the whole $GaAs/Ga_{0.7}Al_{0.3}As/GaAs/Ga_{0.7}Al_{0.3}As$ system. The corresponding peaks in the DOS present a noticeable intensity only for large values of d_1 and in the vicinity of E_3. Recently, Fafard *et al* [2] have observed, in photoreflectance experiments, oscillatory behaviour induced by a barrier layer (called a cap layer) in $GaAs/In_xGa_{1-x}As$ quantum wells, where the effects of the energy levels of a high potential in the vicinity of the quantum well have been studied. Calculations [5] of the probability of finding carriers in the cap layer of the device are derived and present similar behaviour as our DOS calculations, in particular the two latter quantities present sharp peaks in the vicinity of E_3, and outside these resonance peaks goes back down close to zero (see figures 3(d) and 6(a)).

An analysis of the local DOS as a function of the space position x_3 (figure 4) clearly shows the localization properties of the different kinds of state belonging to different

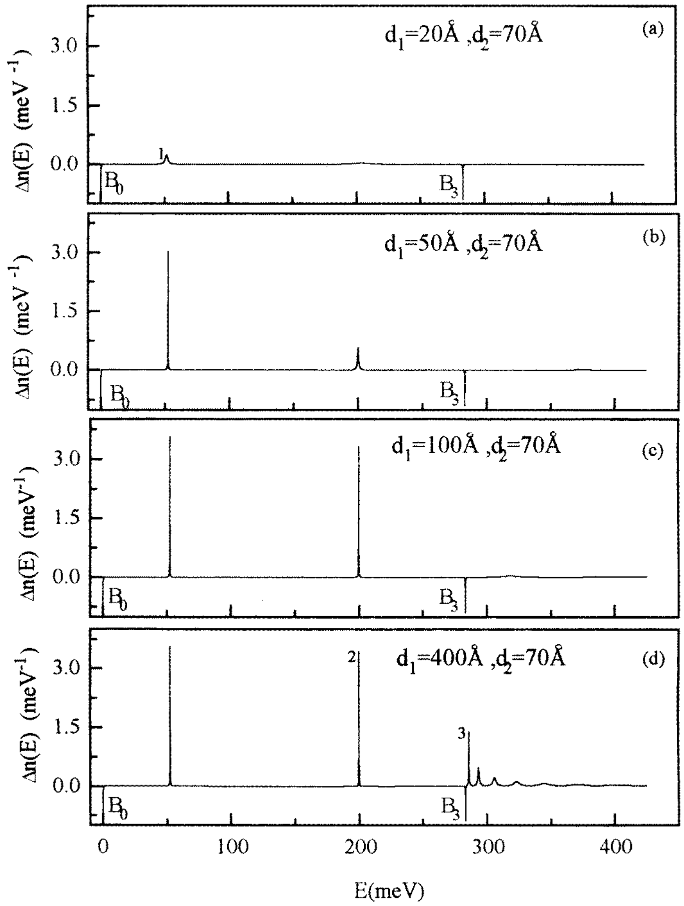

Figure 3. Variation of the DOS as explained in (21) for $d_1 = 20$ Å, 50 Å, 100 Å and 400 Å in figure 2, while d_2 is kept constant ($d_2 = 70$ Å). The antiresonances appearing at $E_0 = 0$ meV and E_3 correspond to delta peaks of weight $-1/4$, resulting from the subtraction of the bulk bands of the GaAs substrate and $Ga_{0.7}Al_{0.3}As$ barrier of infinite extent.

energy range. The local DOS reflects the spatial behaviour of the square modulus of the wave function (i.e., the charge distribution). Figures 4(a) and (b) correspond to the states respectively labelled 1 and 2 in figures 3(a) and 3(d), showing that these resonances are confined in the GaAs well. Moreover, for small thickness of the $Ga_{0.7}Al_{0.3}As$ barrier (figure 3(a)), the interaction between states in the GaAs well and GaAs substrate becomes important and electrons could propagate in the GaAs substrate by tunnelling through the $Ga_{0.7}Al_{0.3}As$ barrier. Figure 4(c) corresponds to the state labelled 3 in figure 3(d), showing that this resonance rather belongs to the barrier layer.

A similar behaviour was found for excitons [16], optical waves [17] and electrons [18, 19] in multiquantum wells, where above-barrier states are localized in the barrier rather than in the well regions.

It is well established that DOS is a much better characteristic of resonant states than transmission rate [11, 20]. However, to our knowledge, there has been no comparison between the DOS and the reflection and transmission phase times to date. In figures 5

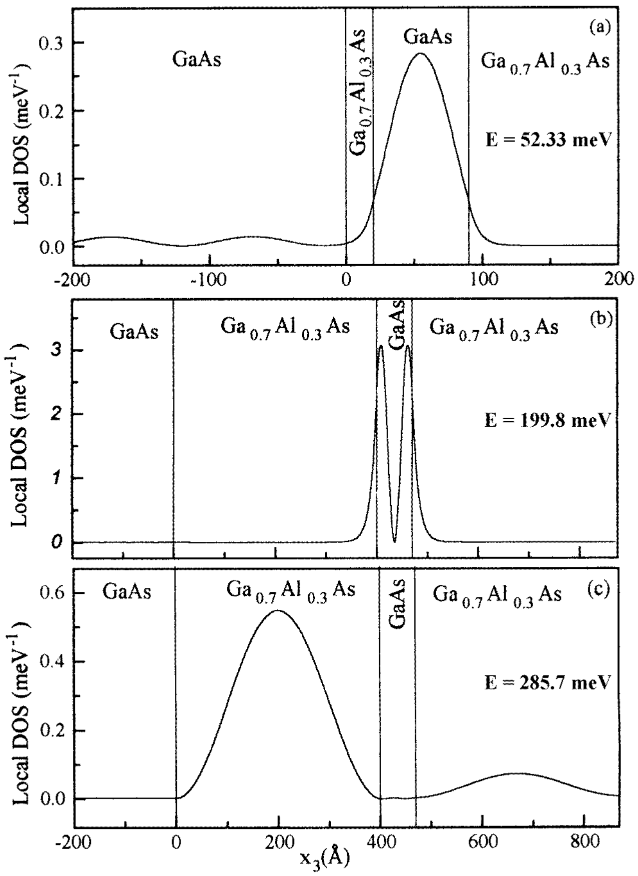

Figure 4. Spatial representation of the local DOS for $E = 52.33$ meV (a), $E = 199.8$ meV (b) and $E = 285.7$ meV (c). These resonances are respectively labelled 1, 2 and 3 in figures 3(a) and 3(b). The space positions of the different interfaces are marked by vertical lines.

and 6, we give a comparison of all the quantities cited above for two different values of the barrier layer: $d_1 = 20$ Å (figure 5) and $d_1 = 400$ Å (figure 6), while the well thickness is kept constant ($d_2 = 70$ Å). Note that the very sharp peaks in the DOS are not broadened artificially by adding a small imaginary part to the energy E, as is the case in figure 3. This is the reason why delta functions do not appear in figure 6(a).

In figure 5(a), two resonances appear below E_3 in the DOS and give the same behaviour as the reflection phase time. Indeed, the halfwidths of the peaks in these two quantities are related to the lifetimes of the resonances. However, the intensity of the peaks in the DOS gives the weight of the resonances, while the intensity of the peaks in the reflection phase time gives the time needed for electron to complete the reflection process. Let us mention that, for energies below E_3, the reflection rate is unity (i.e., the transmission rate is zero), therefore, only the phase time gives us information on the interaction of an incident electron with resonant states confined in the GaAs well.

As mentioned above, for a large value of d_1 (figure 6) and for energies lying below E_3, we find the situation of a classical quantum well sandwiched between two barriers of infinite extent; the resonant states become bound (localized) states: their energies are

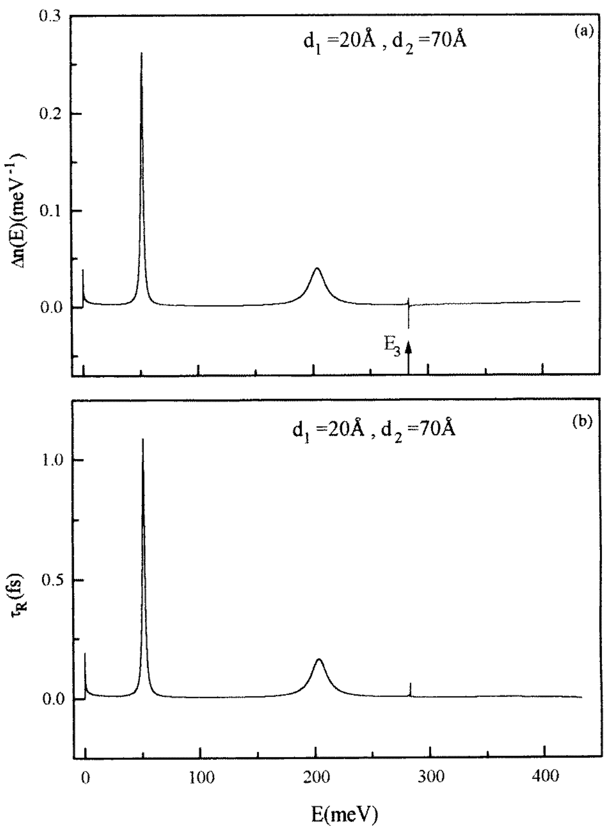

Figure 5. Energy dependence of the DOS (a) and reflected phase time τ_R (b) for $d_1 = 20$ Å and $d_2 = 70$ Å. The arrows indicate the positions of E_0 and E_3 energy levels.

indicated by arrows in the DOS (figure 6(a)). However, for the energy range $E > E_3$, the resonant states depend strongly on the $Ga_{0.7}Al_{0.3}As$ barrier thickness and their intensity decreases with increasing energy. On the other hand, the transmission rate (figure 6(b)) shows sharp peaks with energy positions corresponding to the resonances in figure 6(a); however at high energies the peaks in the DOS vanish, while the peaks in the transmission rate oscillate before they reach unity. An analysis of the phase times of the transmitted and reflected electrons from the GaAs/$Ga_{0.7}Al_{0.3}As$ bilayer, shows that the transmitted and reflected phase times (figures 6(c), (d)) have the same behaviour as the DOS for energies lying above E_3. We remark also that the time needed for an electron to be reflected is almost twice that needed for the transmission. Reflected and transmitted phase times are interpreted as the delay motion of the electrons to appear on the right and left sides of the GaAs/$Ga_{0.7}Al_{0.3}As$ double layers.

Finally, as a matter of completeness, we have also studied the behaviour of the resonant states as a function of the GaAs well layer thickness. Figure 7 presents the variation of the energy of the resonances as a function of the thickness d_2 for a given value of the barrier layer d_1 such that $d_1 = 200$ Å. The resonances lying below E_3 tend asymptotically to the limit of $E_0 = 0$ meV when $d_2 \to \infty$; their intensities in the DOS increase with increasing d_2. However, the peaks of the DOS above E_3 become very weak and probably very difficult to observe experimentally [1].

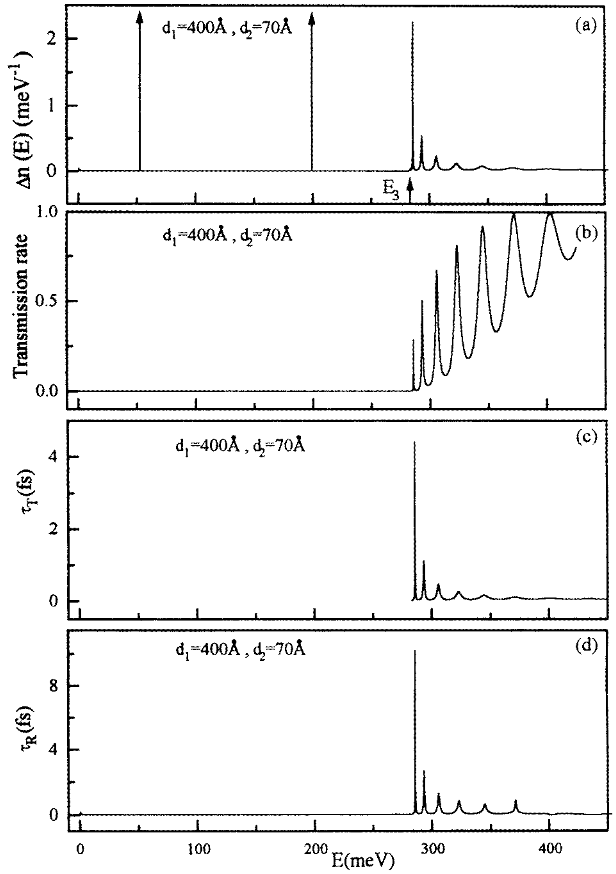

Figure 6. Energy dependence of the DOS (a), transmission rate (b), transmitted phase times τ_T (c) and reflected phase times τ_R (d) for $d_1 = 400$ Å and $d_2 = 70$ Å.

5. Discussion and summary

Our DOS and phase time results revealed a variety of features associated with the interactions of a GaAs substrate bulk states with states of a quantum well. We have shown, in particular, the existence of well defined peaks in the DOS and phase times associated with resonant states in the GaAs well, even though they are in resonance with the bulk states of the GaAs substrate. The intensity of the peaks in the DOS and phase times depend strongly on the width of the barrier separating the well and the substrate. Indeed, the effect of the substrate on resonant states below the barrier appear, essentially, in the broadening of the corresponding peaks in the DOS and phase times for thin barrier layer thickness as the interaction between confined states in the GaAs well and the GaAs substrate is strong. However, for large barrier layer thickness, the resonant states do not feel the effect of the substrate as the interaction between the states in the well and in the substrate become very weak. For energies lying above the barrier, the resonant states become very broadened in the DOS and phase times especially for high energies due to their interaction with the bulk states of both the GaAs substrate and the $Ga_{0.7}Al_{0.3}As$ barrier of infinite extent (figure 1).

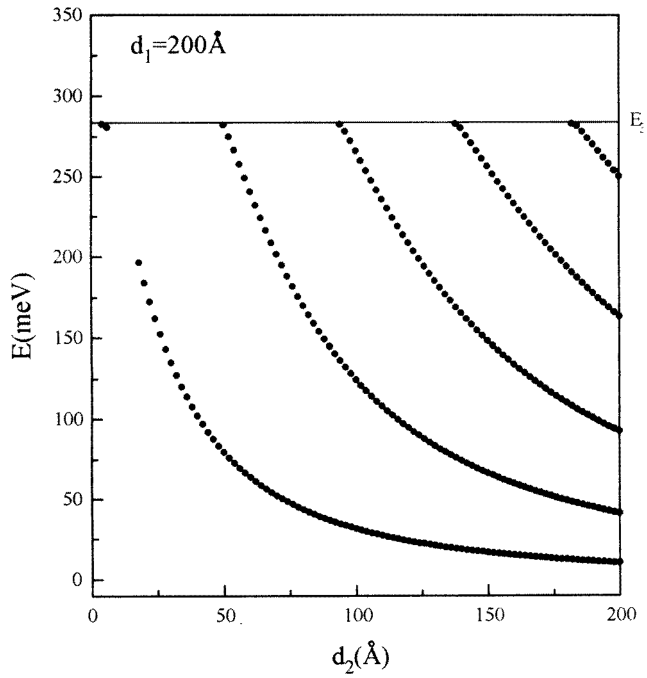

Figure 7. Variation of the energy levels of resonant states, for $d_1 = 200$ Å, as a function of d_2.

Our results reveal also that the peaks in the DOS and phase times present similar behaviour as a function of energy.

In the absence of the GaAs substrate (e.g., for a high substrate potential E_0 as in the case of an AlAs material), the resonant states lying below the barrier become localized (or bounded) states given by the vanishing of the dominator of the Green function (7), with decaying wave functions in the substrate region. However, the above-barrier states ($E_3 < E < E_0$) remain resonant states because of their interaction with the bulk states of the $Ga_{0.7}Al_{0.3}As$ barrier of infinite extent. This latter situation, which is different from ours, is studied in previous works [1–3] where the barrier layer of finite thickness in figure 1 plays the role of a cap layer at the surface of the device. Therefore, substrates on which quantum well structures are grown together with barrier layers separating the substrate and the well should be taken into account for estimating device applications. Our results are in accordance with experimental studies [1–4] showing the necessity of considering the nature and size of the media surrounding a quantum well system.

In summary, we have presented an analytical calculation of the Green functions for electronic energy levels in a single quantum well taking into account the effect of the size and the height of barrier separating the well and the substrate as well as the effect of this latter material (called the buffer layer in experiments) which serves as a support for the device. These complete and closed-form expressions of the Green functions can be used to study any physical property of this structure. This includes the calculation of local and total densities of states and the determination of the dispersion relation for resonant waves in the structure. The Green function approach used in this analysis also enables us to obtain the reflection and transmission rates as well as the corresponding phase times.

The expression of the DOS enables us to derive the dispersion of resonant states (called also leaky waves or quasibounds) in the embedded GaAs/$Ga_{0.7}Al_{0.3}As$ bilayer. Particular attention was devoted to (i) sharp resonant waves confined in the GaAs well, as a consequence of its separation from the GaAs substrate by a $Ga_{0.7}Al_{0.3}As$ barrier of finite thickness, (ii) above-barrier resonant waves propagating in the whole system with an important confinement in the barrier layer. These resonances appear as well defined peaks of the DOS and phase times, with their relative importance being very dependent on the thickness of the barrier and the well layers as well as on the substrate. The experimental observation of the sharp resonances predicted here in such a single quantum well can be possible with photoluminescence [1] and photoreflectance [2] techniques.

Note also the measured time delay of a photon tunnelling through a one-dimensional photonic band material [21]. Let us mention, finally, that similar results to those presented here are found by some authors for transverse [22] and sagittal [23] elastic waves in an adsorbed bilayer on a substrate.

References

[1] Moison J M, Eless K, Houzay F, Marzin J Y, Gérard J M, Barthe F and Bensoussan M 1990 *Phys. Rev.* B **41** 12 945

[2] Fafard S, Fortin E and Roth A P 1992 *Phys. Rev.* B **45** 13 769

[3] Fafard S, Fortin E and Roth A P 1993 *Phys. Rev.* B **47** 10 588

[4] Parks C, Alonso R G, Ramdas A K, Ram-Mohan L R, Dossa D and Melloch M R 1992 *Phys. Rev.* B **45** 14 215

[5] Fafard S 1992 *Phys. Rev.* B **46** 4659

[6] Hauge E H, Falck J P, Fjeldly T A 1987 *Phys. Rev.* B **36** 4203

[7] Hauge E H and Stõveng J A 1989 *Rev. Mod. Phys.* **61** 917

[8] Iannaccone G and Pellegrini B 1994 *Phys. Rev.* B **49** 16 548 and references therein

[9] Landauer R and Martin Th 1994 *Rev. Mod. Phys.* **66** 217

[10] Dobrzynski L 1990 *Surf. Sci. Rep.* **11** 139 and references therein

[11] Trzeciakowski W, Sahu D and George T F 1989 *Phys. Rev.* B **40** 6058

[12] Bahder T B, Bruno J D, Hay R G and Morrison C A 1988 *Phys. Rev.* B **37** 6256

[13] Wigner E P 1955 *Phys. Rev.* **98** 145

[14] Hartman T E 1962 *J. Appl. Phys.* **33** 3427

[15] Ohno H, Mendez E E, Brum J A, Hong J M, Agullo-Rueda F, Chang L L and Esaki L 1990 *Phys. Rev. Lett.* **64** 2555

[16] Zhang F C, Luo N Dai, H, Samarth N, Dobrowolska M, Furdyna J K and Ram-Mohan L R 1992 *Phys. Rev. Lett.* **68** 3220

[17] Bah M L, Akjouj A, El Boudouti E H, Djafari-Rouhani B and Dobrzynski L 1996 *J. Phys.: Condens. Matter* **8** 4171

[18] Jaros M and Wong K B 1984 *J. Phys. C: Solid State Phys.* **17** L765

[19] Babiker M and Ridley B K 1986 *Superlatt. Microstruct.* **2** 287

[20] Bruno J D and Bahder T B 1989 *Phys. Rev.* B **39** 3659

[21] Steinberg A M, Kwiat P G and Chiao R Y 1993 *Phys. Rev. Lett.* **71** 708

[22] Akjouj A, El Boudouti E H, Sylla B, Djafari-Rouhani B and Dobrzynski L 1996 *Solid State Commun.* **97** 611

[23] El Boudouti E H, Djafari-Rouhani B and Akjouj A 1997 *Phys. Rev.* B **55** 4442