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Transmission and escape in finite superlattices with Gaussian modulation

M. de la Luz Silba-Vélez[a], R. Pérez-Álvarez[a], and D.A. Contreras-Solorio[b]
[a]*Universidad Autónoma del Estado de Morelos,*
Ave. Universidad 1001, 62209, Cuernavaca, Morelos, México.
e-mail:svml@uaem.mx; rpa@uaem.mx
[b]*Unidad Académica de Física,*
Universidad Autónoma de Zacatecas. Zacatecas, México.
e-mail: dacs10@yahoo.com.mx

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We study the transmission and escape energies dependent as a function of the electron energy in superlattices where the barriers height is modulated by a Gaussian function and they are compared with those produced by regular superlattices where all the barriers have the same height. We use for the calculations the effective mass approximation using the transfer matrix formalism. For Gaussian systems with 7 and 9 barriers, the transmission coefficient has passbands with almost perfect transmission. The escape energies $E = E_r + i\Gamma$ are situated near these transparency bands but they do not coincide with them and they can be far from the passbands. E_r is the electron energy and Γ describe the width of the states. For these systems the escape states are very wide. In the case of regular systems there are transmission bands which present only resonance peaks with unit value. The escape states are narrow and coincide with these resonances much better than in the case of Gaussian superlattices but the coincidence is not perfect. For 3 barriers where the height of the lateral barriers is reduced gradually, the resonances transform to transparency bands and the width of the escape energies increases. Although there is no coincidence, we associate the increase of width of the escape energies with the formation of transparency bands.

Keywords: Effective mass; transmission; escape; transfer matrix formalism.

Estudiamos la transmisión y energías de escape como función de la energía en superredes donde las alturas de las barreras están moduladas por una función gaussiana y son comparados con los producidos por una superred regular donde todas las alturas de las barreras es la misma. Para los cálculos utilizamos la aproximación de masa efectiva usando el formalismo de matrices de transferencia. Para sistemas gaussianos con 7 y 9 barreras, el coeficiente de transmisión tiene bandas de paso con transmisión casi perfecta. La energías de escape $E = E_r + i\Gamma$ están situadas cerca de las bandas de paso. E_r es la energía del electrón y Γ describe el ancho de los estados. Para estos sistemas los estados de escape son amplios. En el caso de los sistemas regulares existen bandas de transmisión que sólo presentan picos de resonancia con valor unitario. Los estados de escape son estrechos y coinciden con las resonancias mucho mejor que en el caso de superredes gaussianas pero la coincidencia no es perfecta. Para 3 barreras donde la altura de las barreras laterales se reduce gradualmente, las resonancias se convierten a las bandas de transparencia y la anchura de las energías de escape aumenta. Aunque no hay una coincidencia, asociamos el aumento del ancho de las energías de escape con la formación de bandas de transparencia.

Descriptores: Masa efectiva; transmisión; escape; formalismo de matrices de transferencia.

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1. Introduction

At the 70's years, Esaki and Tsu [1] proposed to make artificial semiconductor structures where the charge carriers were confined. First results were obtained confining electrons in two dimensions (quantum wells and superlattices), followed by confining electrons in one and zero dimensions (quantum wires and dots). The necessity to control the optical and electronic properties of semiconductor systems, caused the birth of the heterostructures with a variable number of interfaces [2]. The technological progress in information and communication these last years has had an enormous influence not only in aspects of research but also in the society, [3,4] for example, in lasers designing, information storage and development of devices for saving and producing energy, etc. Nowadays it is usual the access to portable and non-portable personal computers or the usage of cellular telephones which have a lot of services that not long ago were inimaginable. Therefore, it is indispensable to study semiconductor heterostructures in order to understand their fundamental properties. Formerly in the literature the transmission for superlattices with a Gaussian modulation in the barriers or potentials heights has been studied. For these systems, the highest barrier is at the center of the structure and the heights of the adjacent barriers decrease in a Gaussian way toward the ends of the superlattice. These systems have the outstanding characteristic that the transmission spectrum presents transparency bands or passbands with almost perfect transmission, separated by gaps or stopbands where practically there is not transmission at all. We establish, in this work, that these type of structures allow that the electrons can escape more easily from the system, causing that the lifetime of those energy states be short. Therefore, the energy width of the states increases due to the Heisenberg's Uncertainty Principle. The overlap of these energy resonances would cause the rise of the transparency bands. We calculate the transmittance and escape energies of electrons in superlattices with 7 and 9 barriers with Gaussian modulation for the barriers height, and we compare this transmittance with that produced by regular superlattices where all the barriers have the same height. Likewise, we make a study of the transmission and escape energies for a three barriers structure where the height of the lateral barriers is gradually reduced in relation to the central barrier. These structures with Gaussian modulation could be useful as filters where electrons can be transmitted almost totally when their energy corresponds to a transparency band (passband), and rejected if their energy corresponds to a stopband [5-7].

In order to perform the calculations for the systems mentioned above, we rely on the effective mass approximation, using the transfer matrix formalism; this approach is presented in Sec. 2. In Sec. 3 we describe the structures we are interested in. In Sec. 4 we present our results. Finally, in Sec. 5 we formulate our conclusion.

2. Theoretical model

We describe the propagation of electrons with variable mass by means of the Ben Daniel Duke's equation [8-11]

$$-\frac{\hbar^2}{2}\frac{d}{dz}\left[\frac{1}{m(z)}\frac{d\Psi(z)}{dz}\right]+(V(z)-E)\Psi(z)=0, \qquad (1)$$

where $\Psi(z)$ and $\Psi'(z)/m(z)$ are continuous functions. We study one-dimensional systems where the profile for the potential $V_{sys}(z)$ and for the mass $m_{sys}(z)$ is described as

$$V_{sys}(z)=\begin{cases} V_L & (-\infty,z_L) \\ V(z) & (z_L,z_R) \\ V_R & (z_R,+\infty) \end{cases} \qquad (2)$$

$$m_{sys}(z)=\begin{cases} m_L & (-\infty,z_L) \\ m(z) & (z_L,z_R) \\ m_R & (z_R,+\infty). \end{cases} \qquad (3)$$

In other words, we consider a system where at its ends, the potentials and the masses are constant (V_L, V_R, m_L and m_R), while in the intermediate zone the potential $V(z)$ and the mass $m(z)$ are dependent on the position (the growth direction of the heterostructure).

We use the next definition

$$\mathbf{\Psi}(z)=\begin{pmatrix} \psi(z) \\ \frac{\psi'(z)}{m(z)} \end{pmatrix}. \qquad (4)$$

To study the problems of transmission and escape we use the transfer matrix formalism, specifically the called associated transfer matrix (ATM) [12].

According to the potential and mass profiles (Eqs. 2 and 3), the solution of the problem expressed in terms of the ATM, can be written as follows

$$\mathbf{\Psi}(z)=\begin{cases} A\mathbf{E}_L^+(z)+B\mathbf{E}_L^-(z) & z\in(-\infty,z_L) \\ \mathbf{T}(z,z_L)\mathbf{\Psi}(z_L) & z\in(z_L,z_R) \\ C\mathbf{E}_R^+(z)+D\mathbf{E}_R^-(z) & z\in(z_R,+\infty) \end{cases} \qquad (5)$$

$$\mathbf{E}_L^+(z)=\begin{pmatrix} 1 \\ \frac{ik_L}{m_L} \end{pmatrix} e^{ik_L(z-z_L)};$$

$$\mathbf{E}_L^-(z)=\begin{pmatrix} 1 \\ -\frac{ik_L}{m_L} \end{pmatrix} e^{-ik_L(z-z_L)} \qquad (6)$$

$$\mathbf{E}_R^+(z)=\begin{pmatrix} 1 \\ \frac{ik_R}{m_R} \end{pmatrix} e^{ik_R(z-z_R)};$$

$$\mathbf{E}_R^-(z)=\begin{pmatrix} 1 \\ -\frac{ik_R}{m_R} \end{pmatrix} e^{-ik_R(z-z_R)}, \qquad (7)$$

where $\mathbf{T}(z,z_L)$ is the ATM [13] and the magnitudes k_L, k_R are defined by

$$k_L=\sqrt{\frac{2m_L}{\hbar^2}\left(E-V_L\right)} \qquad (8)$$

$$k_R=\sqrt{\frac{2m_R}{\hbar^2}\left(E-V_R\right)}. \qquad (9)$$

The continuity conditions on z_L and z_R gives the matching condition

$$A\mathbf{T}\mathbf{E}_L^+ + B\mathbf{T}\mathbf{E}_L^- = C\mathbf{E}_R^+ + D\mathbf{E}_R^-. \qquad (10)$$

In order to simplify the notation, we write

$$\mathbf{E}_L^\pm \equiv \mathbf{E}_L^\pm(z_L)$$
$$\mathbf{E}_R^\pm \equiv \mathbf{E}_R^\pm(z_R)$$
$$\mathbf{T} \equiv \mathbf{T}(z_R,z_L)\,. \qquad (11)$$

The transmission coefficient is given by the ratio of the probability current for the transmitted wave over that of the incident wave: $T=|j_{\text{trans}}|/|j_{\text{inc}}|$. This coefficient indicates the probability that a particle goes through a barrier due to the tunnel effect [14]. We consider the scattering problem where there is an incident wave from left, other reflected back to the left and a transmitted wave to the right of the structure, which means that $D=0$. The system of equations to solve for obtaining the expression for T is given by Eq. 10. The result is

$$T=\frac{4k_Rk_L}{m_Rm_L\left[\left(T_{21}-\frac{k_Rk_L}{m_Rm_L}T_{12}\right)^2+\left(\frac{k_L}{m_L}T_{22}+\frac{k_R}{m_R}T_{11}\right)^2\right]}. \qquad (12)$$

The reflection coefficient R is obtained in a similar way, or taking into account that $R+T=1$ [15].

The problem of escape is related to having electrons confined in the heterostructure and due to the tunnel effect they leave the system. We consider only outgoing waves, and the coefficients $A = 0$ and $D = 0$ out of the interval (z_L, z_R). Then Eq. 10 gives the transcendental equation [16]

$$\frac{k_R}{m_R} T_{11} + \frac{k_L}{m_L} T_{22} + i \left(T_{21} - \frac{k_R k_L}{m_R m_L} T_{12} \right) = 0. \quad (13)$$

The solutions to Eq. 13 have the form $E = E_r + i\Gamma$, where the real part E_r represents the energy levels while the imaginary part Γ describe the fact that the energy levels are not stationary and they decay.

3. Mass and potential profiles

We have expressions relatively general for the transmission coefficient and for the trascendental equation of the escape problems, in terms of the ATM. To determine the elements of the matrix is necessary to establish the potential and mass profiles in which we are interested. The ATM of the system is obtained using the properties of these matrices [13,17-19]. The first case at we are interested is a superlattice where the height of the barriers V_i are centered at z_i, and modulated by the Gaussian function $V(z) = V_0 \exp\left(-z^2/\sigma^2\right)$, where V_0 is a constant and $\sigma/\sqrt{2}$ is the standard deviation. We present in Fig. 1 the Gaussian profile for a superlattice of 9 barriers. The structure is made of the materials AlGaAs/GaAs. The wells are made of GaAs and the barriers can be built varying the molar fraction x for the alloy $Al_x\, Ga_{1-x}As$. The highest barrier is $V_0 = 0.02425$ Ry and corresponds to $Al_{0.45}Ga_{0.55}As$. Until this value of Al concentration the alloy has direct gap. In order to calculate the concentration x and the electron effective mass in the alloy, we use the crystal virtual approximation [20-22] with

$$V = 0.0539x$$
$$\frac{1}{m_i} = \frac{x_i}{m_A} + \frac{1 - x_i}{m_G}\ , \quad (14)$$

where m_A and m_G are the effective masse for AlAs and GaAs, respectively. It is clear that we have potential and mass piecewise constants, and then the Eq. 1 becomes the Schrödinger equation for each interval.

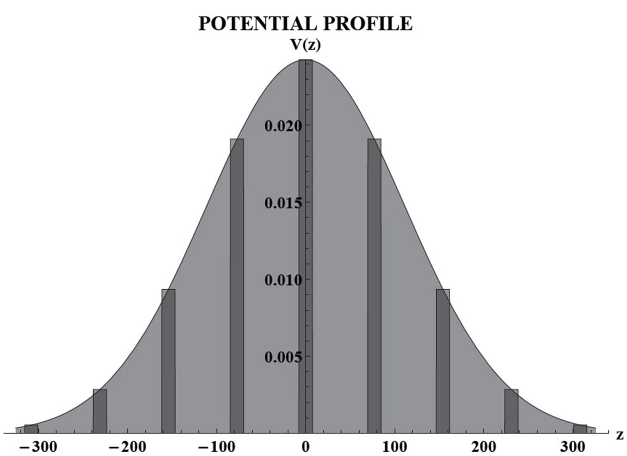

FIGURE 1. Gaussian potential profile. Potential is given in Ry and position in Å.

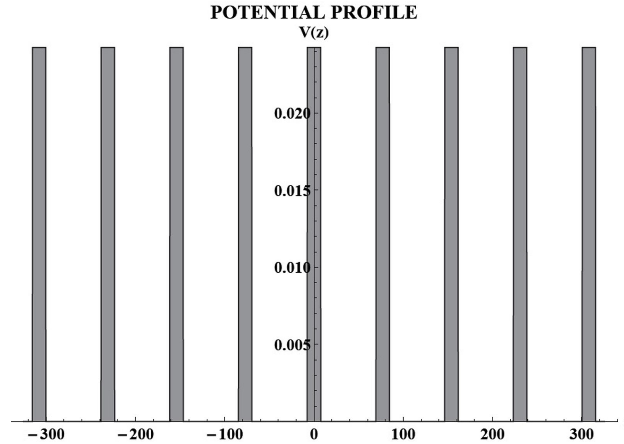

FIGURE 2. Regular potential profile. Potential is given in Ry and position in Å.

A potential with regular or uniform distribution is that made by barriers and wells like that of Fig. 2, that is to say, the potential is constant and is the same for all the barriers. The effective mass is the same for all the barriers but different from that of the wells.

4. Results and discussion

We present in Fig. 3 the transmittance T and the escape energies $E = E_r + i\Gamma$ for a superlattice with 9 barriers whose height has Gaussian modulation. The maximum height for the central barrier is $V_0 = 0.0242542$ Ry. The barriers thickness is $W_b = 15$ Å and the thickness for the wells is $W_w = 62$ Å. The total length for the structure is $L = 631$ Å. We use Eq. 14 in order to find the concentrations x_i and effective masses m_i. We take $m_A = 0.15 m_0$, $m_G = 0.067 m_0$, where m_0 is the free electron mass. The widths $(E_r - (\Gamma/2), E_r + (\Gamma/2))$ associated to each energy E_r are presented as shaded rectangles with different gray

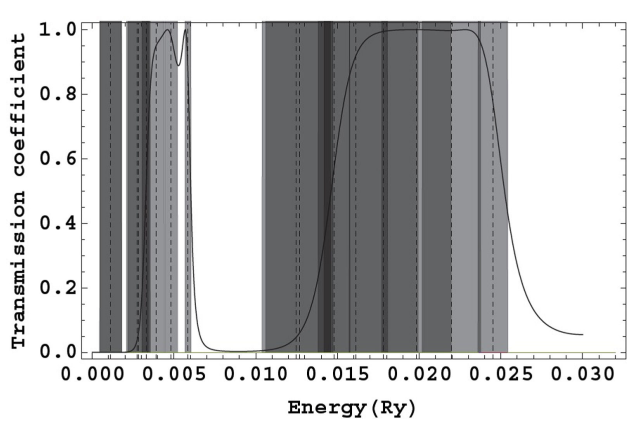

FIGURE 3. T (continuous line) and the escape energies (dashed lines) with their associated width for a Gaussian superlattice with 9 barriers. $W_b = 15$ Å, $W_w = 62$ Å and $L = 631$ Å.

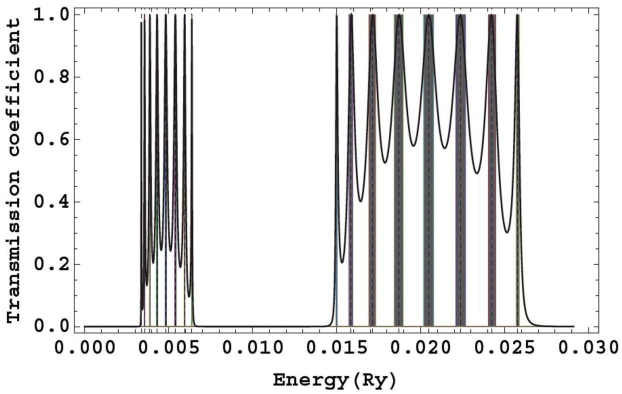

FIGURE 4. T and the escape energies with their associated widths for a 9 barriers regular structure. $W_b = 15$ Å, $W_w = 62$ Å and $L = 631$ Å.

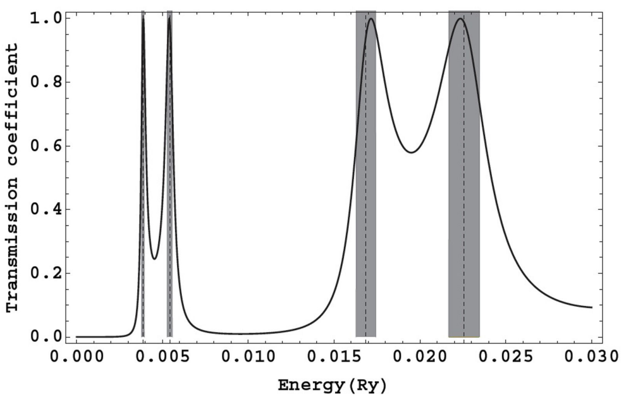

FIGURE 5. T and the escape energies for a three barriers regular structure. $V = 0.0242542$ Ry for the three barriers.

tones. The height of the rectangles has no meaning. The transmitance has two passbands with almost perfect transmission below the highest central barrier, separated by a stopband, and another passband before the first narrower passband. We found 8 escape energies E_r that tend to group in the passbands but no necessarily are inside the passbands. Some E_r can be situated outside of the passband. The escape energies for this Gaussian system have large widths $(E_r - (\Gamma/2), E_r + (\Gamma/2))$, which means that these states have short lifetimes. Figure 4 shows the transmittance and the escape energies for a regular superlattice with 9 barriers with the the same height $V_0 = 0.0242542$ Ry. In this case there are also transmission bands separated by stopbands or gaps where there is no transmission, but the transmission bands consist of narrow transmission resonances. The number of peaks is equal to the number of wells in the structure, in this case, 8 resonances. This corresponds to the splitting of each level of one quantum well in 8 levels. For the regular structure the coincidence between the transmission resonances and the escape energies is much better than in the case of Gaussian superlattices. The escape energies almost coincide with the transmission resonances, but the coincidence is not perfect. The coincidence is almost perfect for the escape energies and resonances at the middle of the transmission

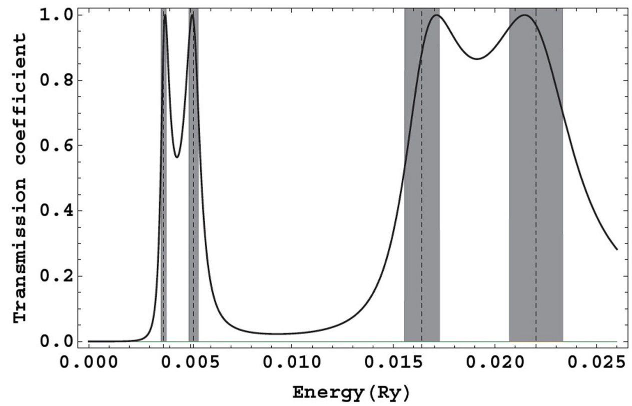

FIGURE 6. T and the escape energies for a three barriers structure. Central barrier $V = 0.0242542$ Ry, lateral barriers $V_l = 0.0187709$ Ry, $W_b = 15$Å and $W_w = 62$Å.

band, and moves away a little for the energies at the extremes of the band. For the regular structure the escape energies are much narrower than for those of the Gaussian superlattice, which means that these states have larger lifetimes. We find that, in general, the values of the escape energies are different from the energy resonances in the transmittance, and this is much more pronounced for Gaussian superlattices than for regular ones. Maksimović also found this fact in his study of propagation of electromagnetic waves in open multilayer systems [23]. They found that the escape frequencies and the transmission resonance frequencies are very similar but are different in general. However in his treatment on resonant tunneling in multilayer structures, Price does not distinguish between escape energies and resonance energies [24]. In the case of a structure with only three barriers, when the structure is regular, with the same height for the three barriers, Fig. 5 shows that the transmittance presents bands with only transmission resonances and the behavior is similar like that of the former regular superlattices with more barriers. Also the width of the escape energies is narrow and the values of the escape energies is near of the resonances. But when the height of the lateral barriers is reduced, Fig. 6 shows that the resonances transform to passbands with high transmission in an interval of energy and the width of the escape energies increases. Likewise, the position of the energies escape moves away from the transmission maxima. Although there is no exact coincidence of the escape energies and the transmission maxima, we associate the large width of the escape energies to the formation of transparency bands.

5. Conclusion

We have calculated the transmittance and escape energies for a finite superlattice where the barriers height follows a Gaussian modulation, and for a regular superlattice where all the barriers have the same height. The Gaussian superlattice have broad intervals of energy or passbands where there is almost total transmission, separated by stopbands where there is no propagation of electrons. For a regular superlattice there are also transmission bands separated by stopbands, but the transmission bands present only narrow resonance peaks. For a Gaussian superlattice the escape energies have very wide linewidths and are situated inside or near the passbands, but they do not necessarily coincide with the passbands. The regular superlattice has escape energies with narrow linewidths, and the values of the escape energies are much nearer to the transmission resonances but in general different from them. In Ref. 25 the spectra of Gaussian and regular structures are studied theoretically and experimentally, and reported its most important features, particularly the shift and resonance broadening; their results agree qualitatively well with those found by us. We associate the large width of the escape energies to the formation of transparency bands. It is important to stress that the mechanism leading to flat transmission is still unknown. Our results are only an approximation of this subject as we perform a comparison of two boundary problems (transmission and escape) on the same potential and mass profiles. It is known that the results of transmittance can be related to the conductance and the results of experiments with two or four probes [26]. Work is in progress on this subject.

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