Matrix method for tunneling in heterostructures: Resonant tunneling in multilayer systems

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We present a scattering-matrix formalism applied for the first time to study electron transmission in extended nonperiodic semiconductor heterostructures. In contrast to transfer-matrix methods, it has the advantage of being stable for all systems without requiring the truncation of the growing exponential states. The method is applied to the study of resonant tunneling in GaAs/$Al_xGa_{1-x}As$ multilayer systems, with the influence of the higher band-structure minima included. The results show that the Γ and the X states give rise to resonances in the transmitted current. Although the positions of the Γ resonances are in qualitative agreement with an analysis using only the Γ minima, the wave function contains significant contributions from the X minima. The X resonances are associated with the AlAs layers. It is concluded that for energies below the conduction-band edge of the barrier material, a single-Γ-state analysis can give qualitative agreement with the many-band analysis, but above the conduction-band edge of an indirect-band-gap barrier, a full many-band model is needed.

INTRODUCTION

The experimental study of vertical transport in semiconductor heterostructures has become more concerned with the quantum nature of the carrier states, with improvements in material-growth techniques. The theoretical modeling of the electron states, and in particular the tunneling properties in multilayer structures, has for the experimentally important situations of nonperiodic systems previously relied on the transfer-matrix method.[1,2] This method, however, is unstable for systems larger than a few hundred angstroms, unless effective-mass theory is used. The origin of the failure is well known[1,2] and lies in the presence of the exponentially growing states in a barrier, whose amplitude varies rapidly in the regions of transmission resonances. The transfer-matrix method treats the growing and the decaying states identically, resulting in the loss of the exponentially decaying wave function during computation, as a result of the presence of the exponentially growing wave function. Various schemes have been proposed[1,2] to deal with this problem. However, they are simply truncation schemes of differing degrees of complexity. For the purpose of resonant tunneling, such schemes are undesirable because, on resonance, the growing and the decaying states contribute equally to the wave function.

In this paper we present an alternative formalism, based on the scattering matrix,[3] in which the physically important eigenstates are allowed to dominate the matrix elements. Consequently, the method remains stable and accurate, even in the limit of large systems and large basis-state sets (Γ, X_1, X_3, etc.). The multistate nature of the tunneling process may therefore be studied accurately, without truncating any of the growing exponential states. Note that the "scattering-matrix" formalisms reported in the literature[4,5] are really "transfer-matrix" methods.

As an example of its application, the method is used to study resonant tunneling in long finite GaAs/$Al_xGa_{1-x}As$ multilayer systems. In particular we are concerned with the effects of the various conduction-band minima and interband transfers. Interwell coupling is considered using triple-barrier systems and more complex structures are also considered.

METHOD

The basis of our method is to calculate the electron states in each of the layers of the multibarrier system and then form a complete eigenstate for the whole system by matching at the interfaces. In practice this is done by using matrices describing the phase shifts across the layers and the scattering at the interfaces. The electronic wave function is obtained from an empirical pseudopotential complex-band-structure method and contains both the Bloch and the evanescent components originating from the various conduction-band minima.[6] This gives a complete set of states, reflecting accurately the band structure of the semiconductor involved. The full details are available in the literature.[6–8] The presence of very fast decaying evanescent modes in such a complete description of the wave function is the cause of the problem with the transfer-matrix technique and, with these states included, we have found that the transfer-matrix method is unstable for systems greater than 5 Å in length.

The scattering matrix[9] which we now present as an alternative couples explicitly the outgoing states to the incoming states of a system. Thus, for a finite N-layer multilayer structure, Fig. 1, the coefficients $\mathbf{a}_N$ and $\mathbf{b}_0$ of the outgoing states are related to the coefficients $\mathbf{a}_0$ and $\mathbf{b}_N$ of the incoming states via the scattering matrix $\mathbf{S}(0,N)$:

$$\begin{bmatrix} \mathbf{a}_N \\ \mathbf{b}_0 \end{bmatrix} = \mathbf{S}(0,N) \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_N \end{bmatrix} . \tag{1a}$$

The equivalent transfer-matrix relationship would be

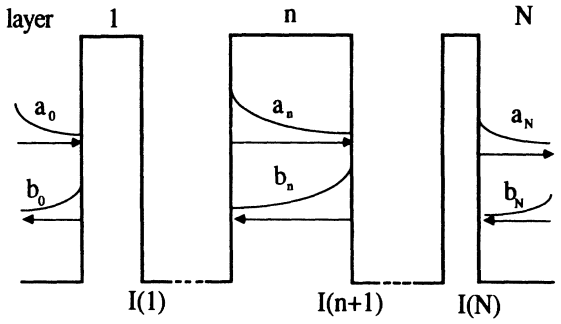

FIG. 1. Schematic diagram of tunneling in an N-layer multilayer system.

$$\begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \end{bmatrix} = \mathbf{T}(0,N) \begin{bmatrix} \mathbf{a}_N \\ \mathbf{b}_N \end{bmatrix} . \tag{1b}$$

$\mathbf{a}$ and $\mathbf{b}$ are the coefficients of the "forward" and the "backward" states, respectively, with the forward states defined as those which propagate or exponentially decay in the positive-z direction and the backward states similarly defined as those which propagate or exponentially decay in the negative-z direction. For the subsystem up to the nth layer, we have

$$\begin{bmatrix} \mathbf{a}_n \\ \mathbf{b}_0 \end{bmatrix} = \mathbf{S}(0,N) \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_n \end{bmatrix} . \tag{2}$$

The matching conditions for the wave functions and derivatives at the $(n+1)$th interface can be expressed in the normal way[4] as a matrix relationship to give

$$\begin{bmatrix} \mathbf{a}_n \\ \mathbf{b}_n \end{bmatrix} = \mathbf{I}(n+1) \begin{bmatrix} \mathbf{a}_{n+1} \\ \mathbf{b}_{n+1} \end{bmatrix} , \tag{3}$$

where $\mathbf{I}(n+1)$ is the interfacial matrix representing the coupling of the barrier and the well eigenstates at the $(n+1)$th interface. The details of the construction of the interface matrix $\mathbf{I}(n+1)$ are given in the literature[4] and depend upon the model used. The coefficients $\mathbf{a}_n$ and $\mathbf{b}_n$ may be eliminated from the above equations to give

$$\begin{bmatrix} -\mathbf{S}_{22}\mathbf{I}_{21} & 1 \\ \mathbf{I}_{11}-\mathbf{S}_{12}\mathbf{I}_{21} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{a}_{n+1} \\ \mathbf{b}_0 \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{21} & \mathbf{S}_{22}\mathbf{I}_{22} \\ \mathbf{S}_{11} & \mathbf{S}_{12}\mathbf{I}_{22}-\mathbf{I}_{12} \end{bmatrix} \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_{n+1} \end{bmatrix} . \tag{4a}$$

The S matrices and the I matrices are, unless otherwise stated, $\mathbf{S}(0,n)$ and $\mathbf{I}(n+1)$, respectively, and the submatrices $\mathbf{S}_{11}$, etc., are defined by writing Eqs. (2) and (3) as

$$\begin{bmatrix} \mathbf{a}_n \\ \mathbf{b}_0 \end{bmatrix} = \begin{bmatrix} \mathbf{S}_{11} & \mathbf{S}_{12} \\ \mathbf{S}_{21} & \mathbf{S}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_n \end{bmatrix}$$

and

$$\begin{bmatrix} \mathbf{a}_n \\ \mathbf{b}_n \end{bmatrix} = \begin{bmatrix} \mathbf{I}_{11} & \mathbf{I}_{12} \\ \mathbf{I}_{21} & \mathbf{I}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{a}_{n+1} \\ \mathbf{b}_{n+1} \end{bmatrix} .$$

From Eq. (4a) the new scattering matrix $\mathbf{S}(0,n+1)$ may be generated:

$$\begin{aligned} \begin{bmatrix} \mathbf{a}_{n+1} \\ \mathbf{b}_0 \end{bmatrix} &= \begin{bmatrix} 0 & (\mathbf{I}_{11}-\mathbf{S}_{12}\mathbf{I}_{21})^{-1} \\ 1 & \mathbf{S}_{22}\mathbf{I}_{21}(\mathbf{I}_{11}-\mathbf{S}_{12}\mathbf{I}_{21})^{-1} \end{bmatrix} \\ &\quad \times \begin{bmatrix} \mathbf{S}_{21} & \mathbf{S}_{22}\mathbf{I}_{22} \\ \mathbf{S}_{11} & \mathbf{S}_{12}\mathbf{I}_{22}-\mathbf{I}_{12} \end{bmatrix} \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_{n+1} \end{bmatrix} \\ &= \mathbf{S}(0,n+1) \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_{n+1} \end{bmatrix} . \end{aligned} \tag{4b}$$

The submatrices of the new scattering matrix $\mathbf{S}(0,n+1)$ are, explicitly,

$$\begin{aligned} \mathbf{S}_{11}(0,n+1) &= (1-\mathbf{I}_{11}^{-1}S_{12}\mathbf{I}_{21})^{-1}\mathbf{I}_{11}^{-1}\mathbf{S}_{11} , \\ \mathbf{S}_{12}(0,n+1) &= (1-\mathbf{I}_{11}^{-1}\mathbf{S}_{12}\mathbf{I}_{21})^{-1}\mathbf{I}_{11}^{-1}(\mathbf{S}_{12}\mathbf{I}_{22}-\mathbf{I}_{12}) , \\ \mathbf{S}_{21}(0,n+1) &= \mathbf{S}_{22}\mathbf{I}_{21}\mathbf{S}_{11}(0,n+1)+\mathbf{S}_{21} , \\ \mathbf{S}_{22}(0,n+1) &= \mathbf{S}_{22}\mathbf{I}_{21}\mathbf{S}_{12}(0,n+1)+\mathbf{S}_{22}\mathbf{I}_{22} . \end{aligned} \tag{4c}$$

Equation (4) expresses the propagation of the wave function through the layers. Starting with the unit matrix for $\mathbf{S}(0,0)$, the successive scattering matrices $\mathbf{S}(0,1),\mathbf{S}(0,2),\ldots,\mathbf{S}(0,n)$ may be calculated, from which the transmission and reflection coefficients can then be obtained using Eq. (1). This iterative procedure is not as easy to use as the transfer-matrix method, which simply reverts to a product of matrices, but the gain in stability more than compensates.

The stability and accuracy of the scattering-matrix method is derived from the separation of the forward and backward states and by doing so, the less localized and the propagating states dominate numerically, the physics of the tunneling process is more faithfully described.

In multiple-barrier systems, the wave function in the intermediate layers is often of interest, since it is needed to give information on properties such as inelastic-scattering-matrix elements, real-space transfers, and oscillator strengths. For large systems, even in the single-tunneling-state limit, which is equivalent to the effective-mass theory limit in terms of numerical stability, the transfer matrix again fails. This is because the coefficients in a given layer are evaluated from those in the previous layers, hence the numerical errors increase with the growing exponentials. To avoid this the scattering-matrix formalism may again be used. For the nth layer of an N-layer system, we have

$$\begin{bmatrix} \mathbf{a}_n \\ \mathbf{b}_0 \end{bmatrix} = \mathbf{S}(0,n) \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_n \end{bmatrix} , \quad \begin{bmatrix} \mathbf{a}_N \\ \mathbf{b}_n \end{bmatrix} = \mathbf{S}(n,N) \begin{bmatrix} \mathbf{a}_n \\ \mathbf{b}_N \end{bmatrix} . \tag{5a}$$

The first of the two equations is simply Eq. (2) restated. The second equation expresses the coupling with the final layer of the system. $\mathbf{a}_N$ and $\mathbf{b}_0$ may be eliminated from Eq. (5a) giving the required intermediate coefficients:

$$\begin{aligned} \mathbf{a}_n &= [1-\mathbf{S}_{12}(0,n)\mathbf{S}_{21}(n,N)]^{-1} \\ &\quad \times [\mathbf{S}_{11}(0,n)\mathbf{a}_0+\mathbf{S}_{12}(0,n)\mathbf{S}_{22}(n,N)\mathbf{b}_N] , \\ \mathbf{b}_n &= [1-\mathbf{S}_{21}(n,N)\mathbf{S}_{12}(0,n)]^{-1} \\ &\quad \times [\mathbf{S}_{21}(n,N)\mathbf{S}_{11}(0,n)\mathbf{a}_0+\mathbf{S}_{22}(n,N)\mathbf{b}_N] . \end{aligned} \tag{5b}$$

This particular form has the advantage that only the initial boundary conditions $\mathbf{a}_0$ and $\mathbf{b}_N$ are required, hence the errors in the coefficients do not propagate from one layer to the next.

Finally, it must be noted that the scattering matrix and its submatrices become singular in the limit of a large system. There is merely a reflection of the physical insignificance of the more localized states. Numerically this makes the rank of the matrices smaller than their actual order and so direct inversions of the submatrices should be avoided.

RESULTS AND DISCUSSIONS

In this section we present the results of a systematic study of electron tunneling in multilayer structures to illustrate the stability of the technique. Two sets of calculations have been performed. The first set is a full multiple-band calculation. It includes 2×25 states (25 forward and 25 backward states) in the electron wave function. This not only includes the Γ and X states, but also those with much shorter decay lengths originating from higher minima. No problems were encountered with the scattering-matrix method even for systems as large as 1000 Å. The transfer-matrix method, however, failed if the exponentially growing wave functions were not truncated for systems larger than 5 Å, and so no results for this approximation are given. In the second set only the Γ state is included in the calculation. However, the pseudopotential complex band structure is used so as to include the nonparabolicities of the energy-momentum dispersion. It is therefore just beyond effective-mass theory in the sense of the envelope function of Altarelli[10] and of Burt.[11] The results of the multistate and single-state analyses are represented throughout by solid and dashed lines, respectively.

The systems, unless otherwise stated, are made up of GaAs wells and AlAs barriers. The band offset has been taken directly from our pseudopotential band structure. This is close to the accepted values[12] and could be adjusted as necessary. However, in this paper we are more concerned with the illustration of the method and the general physical trends. The transmission amplitude is defined as usual to be the ratio between the total transmitted current and the incident current.

Figure 2 shows the effects of varying barrier widths L_B on the transmission amplitude. Results for four symmetric double-barrier structures are presented. The GaAs well width is 56.5 Å for all the structures. The results show two resonances at approximately 70 and 275 meV for the single-state calculation, and approximately 80 and 290 meV for the multistate calculation. These are associated with the GaAs Γ well and arise as a result of the confinement in the GaAs layer. As expected from simple single-state analysis, their positions are essentially independent of the barrier widths. The multistate calculations give slightly higher energies than the single-state calculations for the two resonances. This may be explained by considering the cell-periodic components of the wave functions. The single-state calculation, as in effective-mass theory, assumes that both the GaAs and

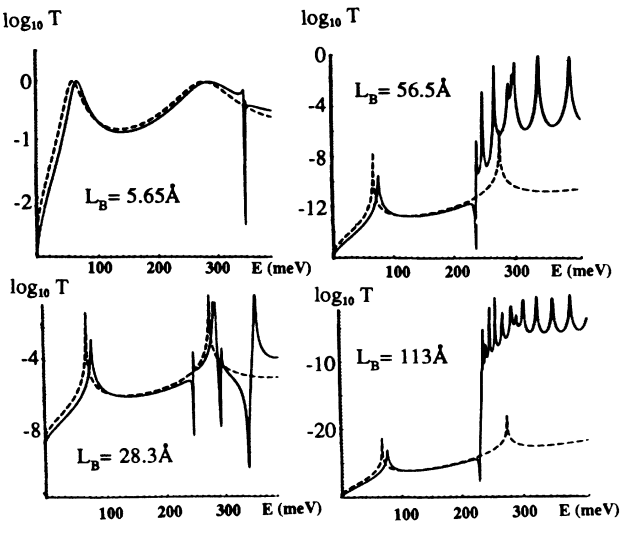

FIG. 2. Logarithmic plots of the transmission amplitudes T as a function of electron energy for four symmetric double-barrier structures with different barrier widths L_B. The dashed line gives the results from the single-state analysis, the solid line represents the results of the multistate analysis.

the AlAs Bloch wave functions have identical cell-periodic components. The multistate calculation, however, includes the cell-periodic components in the matching conditions.[4,7,13] The result is a greater mismatch of the GaAs and the AlAs wave functions, leading to an enhanced confinement of the electron in the GaAs layer. The resonant energies are therefore increased.

The other resonances, observed above the AlAs X-minima energy, are X resonances[14] associated with the potential wells formed with the X minima which, for this system, are located in the AlAs layers.

The effects of the GaAs Γ well widths L_W are examined next. Figure 3 presents the transmission amplitudes for four symmetric double-barrier systems, with barrier widths of 56.5 Å and well widths L_W varying from 5.65 to 113 Å. In the narrowest system, no resonances associated with the GaAs layer are observed. As the GaAs-layer width is increased, Γ-well resonances appear in the transmission amplitude. Their positions from the multistate analysis agree qualitatively, though not quantitatively, with the results of the single-state analysis. Thus, the Γ state determines the positions of the multilayer resonances, regardless of the tunneling electron's energy. The reason for this is because the electron is Γ-like in the GaAs layer and the phase change of the electron, on reflection from the GaAs/AlAs interfaces, is dominated by the scattering of the AlAs Γ state. Since the resonance position is governed by a phase condition,[15] the X contribution to the energy is therefore comparatively small. The positions of the multiple-barrier resonances are therefore a Γ-state property, with the Γ-Γ *band offset* as the appropriate barrier height. However, for energies above the barrier conduction-band edge, the single-state

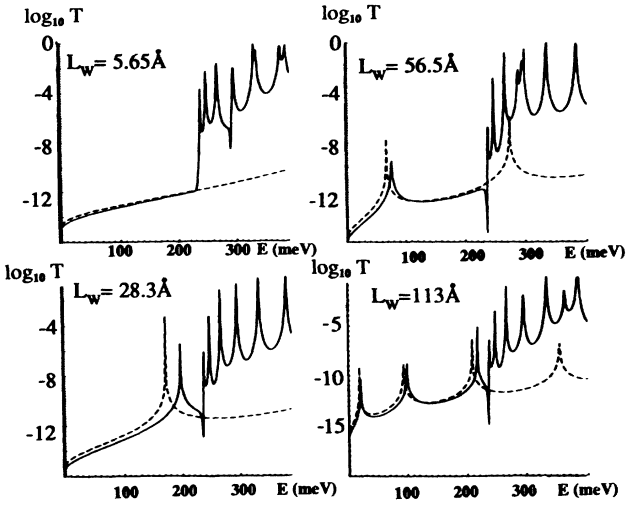

FIG. 3. Logarithmic plots of the transmission amplitudes T as a function of electron energy for four symmetric double-barrier structures with different well widths L_W. The dashed line gives the results from the single-state analysis, the solid line represents the results of the multistate analysis.

transmission is significantly different from the multistate analysis. In addition, the wave functions associated with the two calculations are very different, with significant contribution from the X states to the wave-function amplitude at the interfaces.[16]

We now turn to the effects of interwell coupling. Table I gives the results for a set of symmetric triple-barrier systems. The two outer barriers have fixed widths of 56.5 Å. The degree of interwell coupling is examined via the splitting, ΔE, of the resonant energies. Only the lowest resonance is considered. For a given middle-barrier width L_B the results show the splitting, ΔE, to increase with decreasing well widths, L_W. This is as expected. For narrower wells, the resonances are pushed to higher energies. Consequently, there is a greater leakage of the wave functions into the middle barrier and the interwell coupling is thereby increased. For comparison, the single-state results are also presented. For the wider wells the two sets of calculations agree to within the energy resolution used (0.5 meV). The difference in the narrow-well results are caused by the contributions from the cell-periodic components of the wave functions. The splitting ΔE disappears for the narrowest wells when the coupling barrier's width is greater than 40 Å. For the wider wells, where the coupling is smaller to begin with, the splitting disappears earlier, at about 25 Å.

The nature of the electronic state in the middle barrier is of interest, and in Fig. 4 the percentage contributions of the Γ and X states to the total wave-function amplitude in the middle barrier of a symmetric triple-barrier system are shown. The upper plot is for a middle-barrier width of 28.3 Å. The lower plot is for a middle-barrier width of 113 Å. The results show that for energies below the AlAs X valley, the contribution is almost totally Γ-like. A transition occurs around the AlAs conduction-band edge as intervalley scattering at the interface dominates, and for the wider barrier (the lower plot). This is a sharp transition, with the wave function rapidly becoming purely X-like. In the narrower barrier, the transition occurs over a larger energy range, and a significant Γ contribution remains. Since in the interwell coupling discussed above only the lowest resonance is considered, the results all correspond to electron energies in the band-gap region of the AlAs material. The Γ domination of the AlAs-barrier wave function in this region thus explains the similar splitting from the multistate and single-state calculations. Interwell coupling for the lower resonances is thus a single-state property.

We have also examined asymmetric triple-barrier systems. The energy splittings, ΔE, are given in Table II. The splittings are defined in this case to be the difference between the splitting at infinite separation, that is when $L_B = \infty$, and the value of L_B used. The outer barriers have identical widths of 56.5 Å, the left-hand well is wider by 5.65 Å than the right-hand well. The values of L_W shown are for the right-hand well. Again, the greatest splitting is found in the system with the narrowest wells. The overall magnitude of the splitting is much less than the symmetric situation, which is as expected since the resonance energies in the two wells are not degenerate, and hence the coupling is only a weak perturbation.

So overall, we have found that many aspects of resonant tunneling in multilayer systems can be modeled by a

TABLE I. Energy splitting ΔE for the $n=1$ subband resonance in a symmetric triple-barrier system. L_B denotes different middle-barrier thicknesses and L_W denotes well widths. (Note that the energy resolution is 0.5 meV.)

	Multistate results (meV)			Single-state results (meV)		
L_B (Å) \ L_W	28.3 Å	56.5 Å	84.8 Å	28.3 Å	56.5 Å	84.8 Å
5.65	88.7	33.6	14.5	102.2	33.6	15.0
11.3	51.6	15.0	6.0	49.1	15.0	6.6
17.0	25.0	7.1	2.5	23.5	7.1	3.0
22.6	12.0	3.0	1.0	11.0	3.0	1.0
28.3	6.0	1.5		5.0	1.0	
33.9	3.0			2.5		
39.5	1.0			1.0		
45.2						

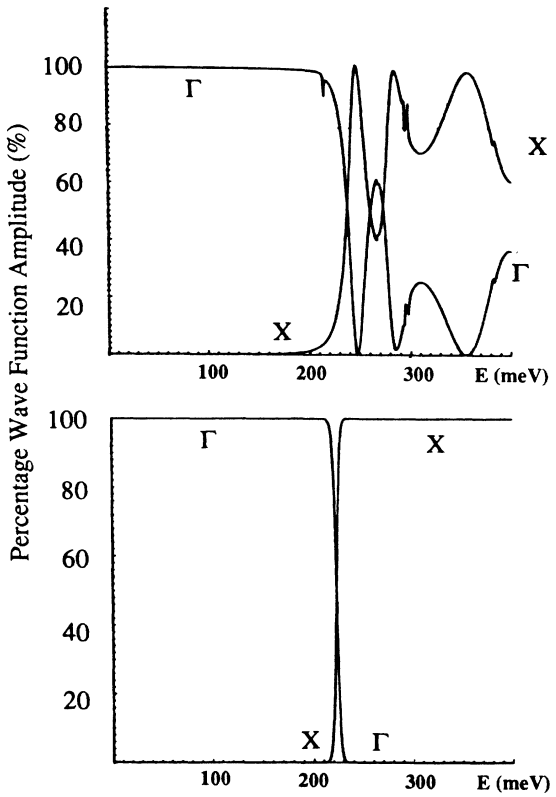

FIG. 4. Percentage contributions of the Γ and X states to the total electron wave-function amplitude in the middle barrier of a triple-barrier system. The upper plot is for a middle barrier 28.3-Å wide, the lower plot is for a middle barrier of 113 Å width.

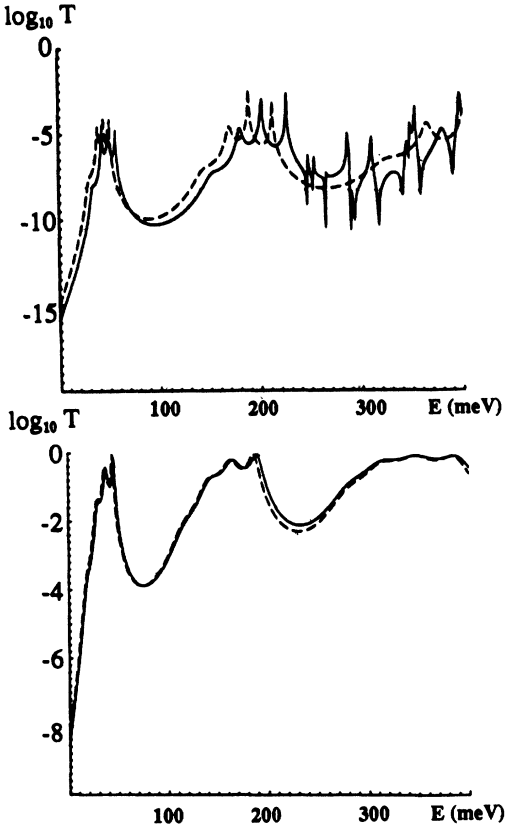

FIG. 5. Logarithmic plots of the transmission amplitudes T as a function of electron energy for asymmetric multibarrier systems. The upper plot is with AlAs barriers, the lower plot is with $Al_{0.30}Ga_{0.70}As$ barriers. The dashed line gives the results from the single-state analysis, the solid line represents the results of the multistate analysis.

single-state picture. There are two types of resonances. The first is associated with the GaAs layers and reflects the multilayer nature of the system. Their positions can be determined to about 10% by considering only the Γ states, with the Γ-Γ band offset as the appropriate barrier height. In the band-gap region of the barrier material, the interwell coupling, as well as the transmission amplitudes, are also single-state properties, again with the Γ-Γ band offset as the appropriate barrier height. The second type of resonance occurs above the AlAs conduction-band edge. They are associated with the AlAs X well and are complicated multistate effects.[14]

We now turn to large multilayer systems that have been studied experimentally[17] but have previously been beyond the scope of microscopic theories. Figure 5 shows the transmission amplitudes for an asymmetric system of four GaAs layers, of widths 67.8, 73.5, 79.1, and 84.8 Å, sandwiched between five $Al_xGa_{1-x}As$ layers, of widths 28.3, 27.6, 17.0, 11.3, and 5.65 Å. The total size of the system is about 500 Å. The upper plot shows the situation with AlAs barriers. Clearly, the transmission amplitude is highly complex, with a large number of

TABLE II. Energy splitting ΔE for the $n=1$ subband in asymmetric triple-barrier systems. L_B denotes middle-barrier thicknesses and L_W denotes well widths. (Note that the energy resolution is 0.5 meV.)

		Multistate results (meV)			Single-state results (meV)		
L_B (Å)	L_W	28.3 Å	56.5 Å	84.8 Å	28.3 Å	56.5 Å	84.8 Å
5.65		61.1	21.0	9.5	60.6	22.0	10.5
11.3		20.0	6.0	3.0	20.0	7.0	3.5
17.0		5.5	1.5	0.5	6.0	2.0	1.0
22.6		1.4			1.5		
28.3		0.5			0.4		
33.9							

resonances. However, the multilayer resonances, associated with the GaAs Γ wells, may be distinguished from the AlAs X-well resonances by comparing with the single-state results. In this system, each GaAs layer has a different width. The resonance energies are therefore nondegenerate. The three sharp peaks and the shoulder associated with each of the two broad resonances, centered at about 45 and 200 meV, thus correspond to Γ resonances in the individual wells. Similarly, above the AlAs conduction-band edge, the large number of AlAs X resonances may also be attributed to resonances in the individual AlAs X wells. The direct-band-gap situation, with $Al_{0.30}Ga_{0.70}As$ barriers, is shown in the lower plot. In this, the transmission is Γ-like, with little qualitative difference from the single-state analysis, even for energies above the barrier X-minima energy.

Figure 6 shows the transmission amplitudes for a similar but symmetric system. The system consists of five periods of 28.5-Å barriers and 67.8-Å wells. The upper plot gives the indirect-band-gap results, with AlAs barriers. The transmission amplitude in this system is much simpler than in the asymmetric system because the resonance energies of the different wells are degenerate, and the layers are sufficiently thick to prevent significant interwell coupling. As before, there are only two Γ-well resonances. The upper one is split due to interwell coupling, leading to a broadened peak. The X-well resonances are at the energies expected from a single AlAs layer. The lower plot shows the direct-band-gap situation, with $Al_{0.30}Ga_{0.70}As$ barriers. The transmission is again dominated by the Γ state. The reduction in the barrier height slightly lowers the energies of the resonances and increases the interwell coupling. Consequently, the resonances are shifted down in energy and even the lowest resonance is significantly broadened.

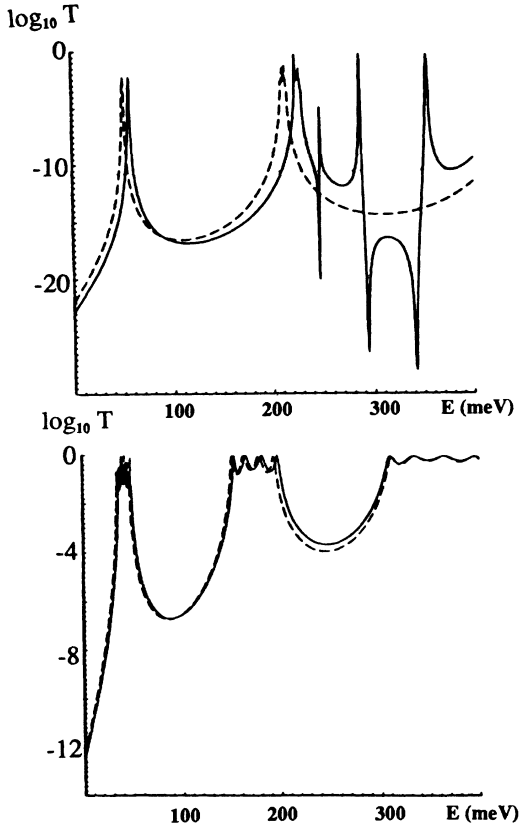

FIG. 6. Logarithmic plots of the transmission amplitudes T as a function of electron energy for symmetric multibarrier systems. The upper plot is with AlAs barriers, the lower plot is with $Al_{0.30}Ga_{0.70}As$ barriers. The dashed line gives the results from the single-state analysis, the solid line represents the results of the multistate analysis.

Throughout, our calculations have assumed coherent tunneling. However, in large systems scattering from alloying effects, impurities and phonons cannot be ignored. Crudely, if the scattering is weak, the effect is simply to introduce an extra phase ϕ_s into the wave function. Within the energy range where the multilayer resonances are single-state properties, the addition of the phase ϕ_s changes the single-state resonance condition[15] to

$$\phi_s+\phi_L+\phi_R+kL=n\pi\ . \tag{6}$$

Here, k is the GaAs Γ-state wave vector, L is the GaAs well width, and ϕ_L and ϕ_R are the phase change on reflection from the left-hand and right-hand interfaces, respectively. Thus, the effect of scattering is to shift the resonance to a new wave vector, $k=k_0-(\phi_s/L)$, where k_0 is the original resonance wave vector, implying that the resonance is not destroyed, but correspondingly shifted in energy. The trends in the transmission we have observed would therefore be expected to remain. The resonance in the transmission current, which is the integrated transmission amplitude of the various k states, would therefore be broadened and the transmitted current peak to valley ratio reduced. Clearly, if the phase shift ϕ_s is not small, such as in inelastic phonon scattering, this analysis is not valid and a sequential tunneling calculation is more appropriate.

Although we have concentrated on the resonance energies, we do wish to stress that the microscopic nature of the states in these systems are *not* single-state-like. There is significant excitation of the evanescent X modes at the interfaces[16] which may significantly change the transmission probability by elastic or inelastic scattering.[18]

CONCLUSIONS

We have presented a new formalism for calculating electron tunneling in large finite multiple-barrier systems, without requiring the use of truncation schemes. The method has been found to remain stable and accurate for large systems.

We have used the method to study the band-structural properties in resonant tunneling in $GaAs/Al_xGa_{1-x}As$ multilayer systems. The results show that the resonance transmissions are readily separated into the GaAs Γ-well resonances and the AlAs X-well resonances. The AlAs X-well resonances are essentially single-layer effects, and do not depend on the multilayer aspects of the systems. The positions of the Γ-well resonances is found to be a

single-state property, with the Γ-Γ band offset as the appropriate barrier height. The magnitude of the transmission amplitude, however, is a multistate property, and depends on the X states' contributions to the barrier wave functions. The same is true for the interwell coupling effects. However, since the resonances of interest tend to have energies below the barrier X minima, where the barrier wave function is largely Γ-like, the single-state picture is reasonably accurate for the energies involved. The cell-periodic components to the wave functions are found to be important. Ignoring it overestimates the overlap of the barrier and well wave functions, leading to a reduced confinement and hence, a lower resonant energy.

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