Resonant tunneling times in superlattice structures

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We present a rigorous and convenient approach for estimating the resonant states from the pole of the scattering matrix (reflection coefficient) in the complex energy plane and for determining the resonant tunneling time from the spacing of the energy doublets arising at resonance. The numerical calculation is much faster than numerical integration of the Schrödinger equation. When we apply this method to the coupling of two identical quantum wells, it is shown that the usual and naive estimation of resonant tunneling time through the Wentzel-Kramers-Brillouin method is invalid. © *1996 American Institute of Physics.* [S0021-8979(96)06310-X]

I. INTRODUCTION

Recently, it has been shown that laser operation is possible in the midwavelength-infrared range (4.2 μm), using resonant tunneling in a superlattice structure.[1,2] Since the population inversion is achieved through resonant tunneling, no pumping is needed in this laser, and different frequencies can be generated relatively easily by the band gap engineering of superlattice structures. Since the earliest suggestion of Kazarinov and Suris in 1971,[3] efforts have continued toward the realization of this type of a laser. These studies became more extensive[4–6] after the development of modern crystal growth technologies such as molecular-beam-epitaxy (MBE) or metalorganic-chemical-vapor-deposition (MOCVD), which have afforded control of material growth on an atomic scale. In 1989, Helm *et al.*, first demonstrated the emission of infrared radiation at 110, 70, and 50 μm, using structures with 5–6 subbands in a well.[7] From these experiments, we suggested[8] that emission at 3–5 μm should be also possible, due to the high (6–7 times) relative efficiencies at these frequencies. Several opposing views[7] were also presented on the possibility of achieving population inversion from this scheme. Although laser operation has recently been demonstrated, even now the theoretical understanding of the mechanism is not complete. In this paper, we present a basis for the understanding of population inversion in a quantum cascade laser by considering how to estimate the resonant tunneling time for electrons between wells in superlattice structures as opposed to the tunneling time through the entire structure or the traversal time for an isolated barrier.[9] Our definition of tunneling time corresponds to the lifetime of the resonant state as defined by Luryi[10] which we called resonant tunneling time throughout the calculations. This will serve as a starting point for the optimization of such IR lasers.

In principle, it is possible to find the resonant tunneling time in superlattice structures by integrating the appropriate time independent Schrödinger equation with respect to time as was done by Juang.[11] However, this is extremely time-consuming, and is not appropriate for device design, where numerous parameters and bias conditions need to be tested, as the resonance depends critically on the applied voltage. Previous workers have conventionally used the Wentzel-Kramers-Brillouin (WKB) method to find the transmission coefficient of carriers through the first relevant barrier. In the classical sense, this gives an estimate of the resonant tunneling time obtained from the number of carrier collisions with the barrier per unit time. As will be shown later, this approach does not fully incorporate the quantum nature of resonance, and does not produce a correct estimation. It predicts a higher transmission at biases beyond resonance which does not agree with experimental results,[12,13] while also seriously overestimating the resonant tunneling time. To make a correct evaluation, it is crucial to use the whole potential profile properly. This means that the neighboring wells and barriers as well as the immediate transparent barrier should be included, and in cases where the more distant wells and barriers have some influence, these should also be considered. Therefore, it is evident that a reasonable answer cannot be obtained from the conventional approach, where only the first well and barrier are included. To deal with several wells and barriers simultaneously and effectively, we use the complex representation method for the energy, or complex energy method—CEM (for short) to indicate both the energy levels and the lifetimes for the metastable states of a system at the same time.[14,15] This method[16] of calculating the energy levels and lifetimes from poles in the complex energy has already been applied in proposed emitter structures.[6] An alternate approach that has been recently suggested for the evaluation of energy levels is the use of a matrix diagonalization method.[17]

II. ENERGY AND LIFETIME FROM COMPLEX ENERGY METHOD

A localized electron in a dc biased superlattice is bound on the emitter side (left side in Fig. 1) by sequentially increasing potential barriers. However an electron can penetrate toward the collector side. The confinement time, or the lifetime of an electron, is determined by the number of barriers it must tunnel through to reach an unbound state. Previous studies by Helm *et al.*[18] provide an experimental indication that the potential inside a well is flat. The step potential across the barrier in the proposed model is an approximation to the real case in which it would be trapezoidal. Usually, dividing barrier regions into about 10 segments is sufficient to simulate the real situation.[19] The lifetime can be

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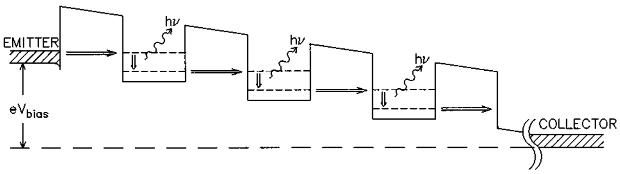

FIG. 1. Biased multiple quantum well heterostructure where electrons cascade down through the series of energy levels associated with the quantum wells and generate radiation.

determined from the scattering of a left incident incoming wave (depicted at the right of Fig. 2). This wave is bound to undergo a total reflection, since a barrier will eventually become higher than the incident energy. Therefore the reflection coefficient R can be expressed as

$$R = e^{i\phi(E)}, \tag{1}$$

where the phase shift $\phi(E)$ is real. Wigner[20] expressed the time delay involved in this scattering as

$$t_{\text{delay}} = \hbar \frac{d\phi(E)}{dE}. \tag{2}$$

By plotting this time delay versus energy, the resonance states could be identified, which correspond to the peaks in time delay, and one could determine the lifetime of those states from the full-width-at-half-maximum of the peaks. However, this is again a cumbersome approach. Here we suggest finding a pole in the reflection coefficient (the *S*-matrix for this case) in the complex energy plane, which is analytic in nature, and a much faster way to obtain the resonance states and their lifetimes. We assume a pole of the form

$$E = E_0 - i\Gamma/2, \tag{3}$$

where E_0 is the resonance energy. This tells us that the pole should be found in the second Riemann sheet of $R(E)$. Generally a pole in the *S*-matrix defines a bound state. The negative imaginary part indicates that it is a decaying bound state

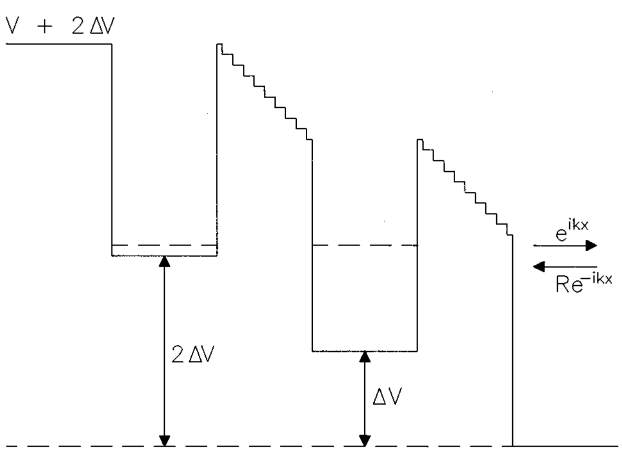

FIG. 2. Proposed potential model for the estimation of resonant tunneling time in a cascade process.

(metastable state). Particles will be lost in time as $\sim e^{-\Gamma t}$.[21] Therefore, the lifetime of a metastable state is given by

$$\Delta t = \hbar/\Gamma. \tag{4}$$

Physically the pole in $R(E)$ means that there can be a reflected wave (the right outgoing wave in our case) with zero incident wave (no left input).[21] This is exactly what happens in a real situation. Equivalently one may impose the outgoing wave boundary condition outside the rightmost barrier.[22] This gives a practical way to find a pole in $R(E)$. For any arbitrary step potential we evaluate the coefficients of right- and left-propagating waves (A_n and B_n, respectively) in each well or barrier region recursively starting from the leftmost region, and set the coefficient of the incoming wave in the rightmost region to zero. The coefficients A_n and B_n are related through the transfer matrix at the nth interface as follows

$$\begin{pmatrix} A_{n+1} \\ B_{n+1} \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} e^{k_n d_n} & e^{-k_n d_n} \\ \dfrac{k_n}{k_{n+1}} e^{k_n d_n} & -\dfrac{k_n}{k_{n+1}} e^{-k_n d_n} \end{pmatrix} \times \begin{pmatrix} A_n \\ B_n \end{pmatrix}, \tag{5}$$

with d_n the thickness for the nth region, V_n the potential in the nth region, and $k_n = \sqrt{2m(V_n - E)}/\hbar$. Notice here that k_n is a complex number. Then the condition for a pole is

$$A_1 = 1, \quad B_1 = 0, \quad B_N = 0, \tag{6}$$

with 1 and N referring to the left- and rightmost regions respectively. This is a simple and rapid process to achieve in a computer program. The solutions are found numerically, using the subroutine ZANLYT in IMSL. Although all variables are declared to be double precision to increase the accuracy, the calculation is almost instantaneous ($\sim$30 ms) for one set of parameters even with a personal computer (Gateway Pentium 90 MHz), showing the efficiency of our approach.

We first apply this method to the simplest single-well case. The result shown in Fig. 3(a) is the evaluation done for a GaAs/AlGaAs system. The number in parentheses indicates the lifetime of the corresponding metastable state. This lifetime agrees with that from the conventional WKB approach and from a dynamic path integral approach. To illustrate that we have found the energy levels correctly from this method we have also shown the corresponding bound case results on the same figure for comparison. We believe these consistencies indicate the validity of our approach.

III. LIFETIMES AT RESONANCE FOR GaAs/AlGaAs SYSTEM

We begin our analysis of resonance with the case of two coupled unbiased bound quantum wells, as indicated in Fig. 3(f). This will be used as a reference system to deduce the transit time in the superlattice structure in the following

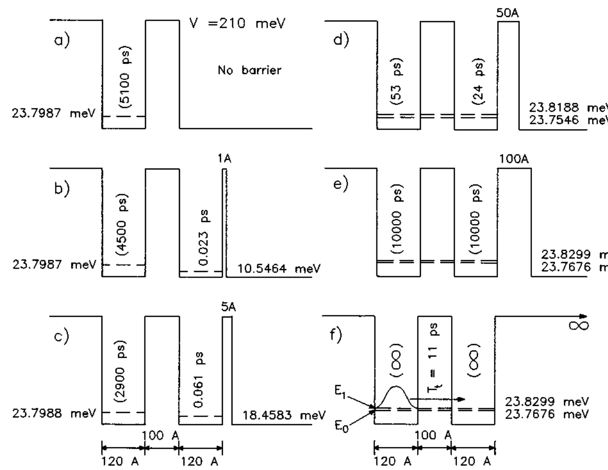

FIG. 3. The energy levels and lifetimes for the metastable states of a GaAs/AlGaAs (a) single quantum well with one transparent barrier, estimated from the CEM, and when a second barrier is added with thickness (b) 1, (c) 5, (d) 50, (e) 100 Å, and (f) ∞ (two coupled bound quantum wells). We also pictorially illustrate a wave packet initially localized in the left quantum well, the mean energy of which is ~23.8 meV. The characteristic resonant tunneling time of this wave packet between the wells is 11 ps for the given parameters.

work. From the standard approach, the energy levels of the ground state and the first excited state of the system are found from

$$\cot(kw) = \frac{1}{2}\left(\frac{k}{K} - \frac{K}{k}\right) \pm \frac{1}{2}\left(\frac{k}{K} + \frac{K}{k}\right) e^{-Kb}$$

$$(+\text{: ground state}, -\text{: first excited state}), \qquad (7)$$

where w is the width of the quantum well, b the thickness of the middle transparent barrier, k, K are the wave numbers in the quantum well and in the barrier, respectively. Now we take Ψ_L and Ψ_R as the wave packet localized in the left and right quantum well respectively. If we start the tunneling system in Ψ_L at the time t=0 and let it evolve, the wave packet would leak into the right quantum well and become Ψ_R at some time, and then leak back into the left quantum well to become Ψ_L again, i.e., the wave packet oscillates between the wells. The characteristic time for this tunneling is known as

$$T_t = \frac{\hbar}{\Delta E} \qquad (8)$$

with ΔE the spacing of the energy doublet in the coupled system. For a GaAs/AlGaAs system with $w = 120$ Å, $b = 100$ Å, and barrier height $V = 210$ meV, the resonant tunneling time T_t is estimated to be 11 ps. This number is much different from the value 5100 ps shown in Fig. 3(a), which is the tunneling time for a similar energy wave packet through a single barrier of same height and width. To understand this issue, we calculate the tunneling times for the systems shown in Figs. 3(b)–3(e), where we place a second barrier behind the first barrier, of the same height as the first one but of different width. We make use of Eq. (5) (with the conditions in Eq. (6)) to calculate the energy eigenvalues and lifetimes of the metastable states. The results are shown in the Table I. When $b_2 = 0$, we simply reproduce the single quantum well results of Fig. 3(a), and can check the accuracy of our numerical program. We take some important results out of Table I and present them in Fig. 3. In Fig. 3(b), where we show the case for $b_2 = 1$ Å, the energy levels and the lifetimes of the metastable states of each well are almost the same as those for independent single quantum wells with the same transparent barriers. This is because the energy levels of each well are so different that minimal coupling is made between them. When $b_2 = 5$ Å (Fig. 3(c)), the metastable state in one well starts to be influenced by the other. The well states are now weakly coupled leading to a reduction in the lifetime of the inner state. In Fig. 3(d) ($b_2 = 50$ Å), the apparent outer well exerts an appreciable effect on the inner well. The two wells are now strongly coupled and start approaching resonance. We notice this from the similarity of the escape times of the two energy levels. However, the relatively large difference between the lifetimes indicates that the resonance is not yet complete. When $b_2 = 100$ Å (Fig. 3(e)), the lifetimes of the two metastable states are almost equal to each other and about twice that of the single quantum well result (Fig. 3(a)). The energy levels are almost the same as the bound case results of Fig. 3(f) to the fourth decimal place. This also indicates the corresponding energy eigenfunctions should be very close to the bound case ones

TABLE I. Results for the double barrier structure as shown in Fig. 3. Here E_0 and E_1 are the energy levels, T_0 and T_1 are the lifetimes of the ground and first excited states respectively and T_t is the resonant tunneling time of a wave packet between the wells at resonance. The resonant tunneling times (T_t) are given as 10.56 and 10.26 ps for illustrative purposes. Elsewhere the numbers are rounded off.

b_2 (Å)	E_0 (meV)	E_1 (meV)	T_0 (ps)	T_1 (ps)	T_t (ps)
0		23.7987		5100	
1	10.5464	23.7987	0.023	4500	
5	18.4583	23.7988	0.061	2900	
10	21.1702	23.7989	0.14	1600	
20	23.0280	23.7994	0.50	520	
30	23.5565	23.8011	1.7	170	
50	23.7546	23.8188	24	53	10.26
70	23.7664	23.8287	320	340	10.56
100	23.7676	23.8299	10000	10000	10.56
130	23.7676	23.8299	320000	310000	10.56
∞	23.7676	23.8299	∞	∞	10.56

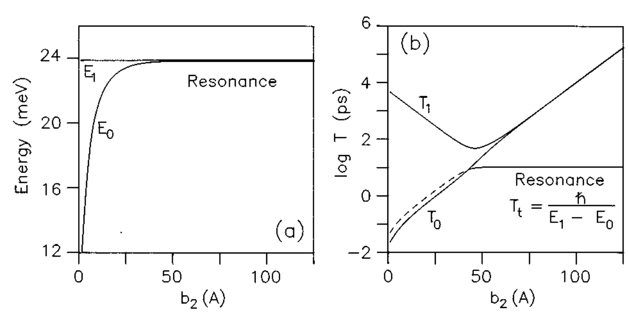

FIG. 4. (a) The energy levels E_1 and E_0 in the double barrier system and (b) the corresponding lifetimes of the metastable states T_1 and T_0 plotted vs the second barrier thickness b_2. The two energy levels come into resonance at $b_2 \sim 50$ Å. Also shown in (b) as a heavy line is the tunneling time for the middle barrier calculated from Eq. (9) with the dashed portion indicating a nonresonant state and the solid portion corresponding to resonance.

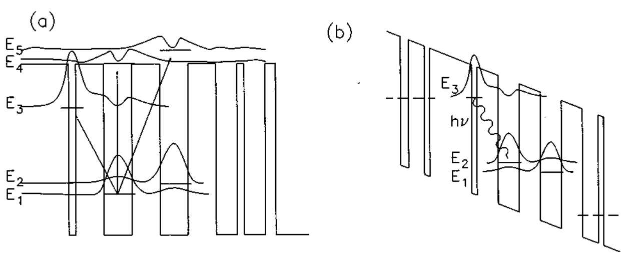

FIG. 5. The quantum cascade laser, reported by Faist *et al.* (Ref. 1). (a) The unbiased case with the arrows showing the transitions $E_1 - E_3$, $E_1 - E_4$ and $E_1 - E_5$. The emission observed is from the $E_1 - E_3$ transition. (b) The biased case with the dashed lines indicating the effective conduction band edge in the injection region. The wavy line indicates the photon-assisted tunneling transition responsible for the electroluminesence.

at this barrier thickness. As we increase further the second barrier width, the energy level results become closer to the bound case results. The corresponding curves for the energy levels and the escape times are shown in Fig. 4. From this, we can see that resonance begins at $b_2 \sim 50$ Å and continues to $b_2 = \infty$. Therefore at $b_2 \geqslant 50$ Å, the energy eigenfunctions and the transit time through the transparent barrier should be close to the bound case ones. We interpret these results as follows. When the metastable state of the outside well is distinct and the energy level matches that of the inside well, this state resonates with the inside state and forms a doublet. We extract from the bound case results the resonant tunneling time of this coupled system between the wells as

$$T_t = \frac{\hbar}{E_1 - E_0}, \tag{9}$$

with $E_1 - E_0$ again the spacing of the energy doublet. This analysis shows the resonant tunneling time, in the example of Fig. 3(e), should be 11 ps for a wave packet of energy ~ 23.8 meV localized in the left quantum well, although the conventional way would predict 5100 ps. We believe that this fast resonant tunneling time should assist in achieving population inversion.

Analyzing the case of a quantum cascade laser reported by Faist *et al.*,[1] under zero bias, we have distinct states E_1 and E_2, which are pretty well localized in the second well and the third well respectively (Fig. 5(a)). When enough bias is applied, the energy level of the second well becomes higher than that of the third well (Fig. 5(b)). In between we have a resonance and there is a minimum energy difference of these two energy levels. Faist *et al.* reported this value to be ~ 20 meV. Our approach resulted in 21 meV for this. What happens at this moment is the two well-localized states get mixed and the middle barrier becomes transparent. We can assume outside barriers for the second and the third well are still distinct, unless the energy levels of these wells resonate with those of other wells. This situation resembles the case which we have just analyzed. Therefore, we claim that the resonant tunneling time for this structure is $\hbar/20$ meV ~ 0.05 ps, rather than the usual assumption of ~ 1 ps.

IV. CONCLUSION

A conceptually rigorous, easy to implement, novel approach involving a pole in the complex energy plane has been used in estimating resonant tunneling times. We analyzed systematically the resonance of double quantum wells with one opaque and two transparent barriers. From this study we suggest a new and convenient way of estimating the resonant tunneling time in superlattice structures. Based on the similarities on escape times and the relatively constant energy separation of the two levels we determined the conditions for a two barrier system under which the time for electrons to tunnel between wells (resonant tunneling time) can be determined using the isolated coupled well model. These systematic analyses show the conventional approach, which uses the WKB method to find the tunneling coefficient and makes a semiclassical estimation, could be off by a factor of several hundred. In conclusion, the correct estimation of energy level and the resonant tunneling time may, depending on experimental studies, be the starting point of the optimization of a quantum cascade laser.

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