Lifetime Analysis of Quasistationary States in Open Superlattices

Ming-Chieh Lin
Department of Physics
Fu Jen University
510 Chung Cheng Rd , Hsinchuang , Taipei Hsien 24205,
Taiwan, R. O. C.

Abstract: - A complex eigen-energy method is presented to investigate lifetimes of the quasistationary states in open quantum heterostructures, open superlattices. The transfer matrix approach is employed to discretize the conduction-band profile of the heterostructure and form a dispersion equation whose zeros correspond to the complex eigen-energies. The quasistationary states are extracted numerically in the complex plane by Newton's method. Both the energy level and the lifetime of the quasistationary state are obtained simutaneously. The method has been proved numerically efficient and accurate by comparing with some results of the APM approach.The differences in lifetime between the quasistationary states in the open superlattices can be easily realized as all the wave functions are specially adjusted to form the relative probability density distributions.

Key-Words: - Lifetime, quasistationary states, complex eigen-energy, transfer matrix, open superlattices

1 Introduction

Resonant phenomena through quantum heterostructures have been the subject of intense scientific research. These phenomena are very important in the design of today's quantum devices such as lasers [1], electro-absorption modulators [2], photodetectors [3], and high-frequency negative-differential resistivity tunneling, and quantum interference devices [4,5]. In general, these devices are complex multiple quantum wells and their performance depends on the characteristics of quantum resonances therein, ie., the electron eigen-energy levels E and their corresponding lifetimes τ, the time that electrons remain confined inside the heterostructure at the given eigen-energy. The fastest possible time response of the device is dictated by the lifetime of its quasistationary state. A complex eigen-energy approach to the (E, τ) determination is the numerical solution of Schrödinger equation in the complex plane. The real part of the complex solution corresponds to E and the imaginary part corresponds to $-\hbar/2\tau$ [6]. In multiple quantum wells, the barriers are thick enough that the wave functions in the neighboring wells do not overlap. In contrast, coupled quantum wells (CQWs), or superlattices, have thin barriers so the electronic wave functions overlap. Superlattices and their transport properties were first investigated by Esaki and Tsu [7]. They predicted negative differential conductance associated with electrons transfer into the negative mass regions of the minizone and Bloch oscillations. Kazarinov and Suris theoretically studied the current-voltage (I-V) characteristic of multiple quantum-well structures with weak coupling between wells and predicted the existence of peaks corresponding to resonant tunneling (RT) between the ground and excited states of adjacent wells [8,9]. Calculations of RT through multiple barriers, CQWs, were also presented by Tsu and Esaki [10], and they found that there would be an (n-1)-fold degeneracy splitting for n barriers, (n-1) CQWs, followed by the observation of RT through double barriers [11]. Esaki and Chang observed oscillatory conductance along the superlattice axis in an AlAs/GaAs multiplayer unipolar structure [12]. In recent decades, owing to the advancement of modern crystal-growth techniques and computers, the quantum heterostructures have been extensively studied via experiments and simulations. For quasistationary states determination, one can select one of the methods including the WKB approach [13], the projected Green's function method [14] and four numerical methods, namely the argument principle method (APM) [15], the perturbed wavevector method [16], the quantum reflection pole method [17], and the modified density of states method [18,19]. The later four numerical methods are capable of determining the quasistationary-state eigen-energies and their lifetimes in quantum heterostructures having arbitrary potential profiles and shown to both numerically efficient and accurate [20]. All of these solve the time-independent effective mass equation, using the transfer matrix approach to discretize the conduction-band profile.

In the present paper, the differences in lifetime between the quasistationary states in open superlattices are concerned. A complex eigen-energy method is employed to investigate the quasistationary states, and the transfer matrix approach is used to discretize the conduction-band profile of the heterostructure and form a dispersion equation whose zeros correspond to the complex eigen-energies. Both the energy levels and the corresponding lifetimes are extracted numerically in the complex plane by Newton's method (NM). The numerical method is proved useful by comparing with some results of the APM approach, which is one of the best numerical methods currently being used [20]. Furthermore, the differences in lifetime between the quasibound states in superlattices can be easily realized as all the wave functions are specially adjusted to form the relative probability density distributions.

2 Formulation

The system of superlattices considered here is an n-barrier quantum heterostructure. The potential profile of a five-barrier four-well case is schematically illustrated in Fig. 1, where the right- and left-hand contacts correspond to pure GaAs, periodically introduced $Al_{0.5}Ga_{0.5}As$ layers give rise to regions having a barrier height of approximately 0.5 eV. The barrier and well widths are 20 Å and 50 Å, respectively, and the effective mass within each region is taken into account via $(0.067+0.083x)m_0$. By symmetry, the Hamiltonian can be split into transverse and longitudinal parts, and the problem can be simplified as solving the time-independent single-band effective mass equation with complex eigenenergies $\hat{E}$ along z direction,

$$-\frac{d}{dz}\left[\frac{1}{m^*(z)}\frac{d\psi(z,t)}{dz}\right]+\frac{2}{\hbar^2}\left[\hat{E}-V(z,t)\right]\psi(z,t)=0, \tag{1}$$

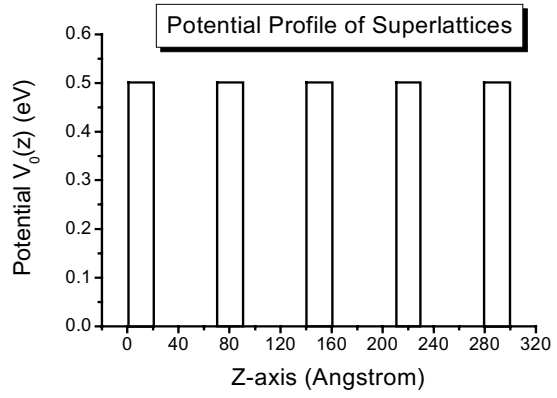

Figure 1 Schematic view of the potential profile of the system of superlattices, a five-barrier four-well quantum heterostructure.

where the longitudinal complex eigen-energies $\hat{E}$ are complex numbers, i.e. $\hat{E}=E_R-iE_I$. The lifetime is $\tau=\hbar/(2E_I)$. Transfer matrix approach is employed to discretize the conduction-band profile of the heterostructure. For an n-barrier open superlattice, $V(z,0_-)$, $V(z,0_+)$ and $m^*(z)$ can be divided into p=1, 2, ...,(2n+1) layers with a piecewise constant potential energy V_p and constant effective mass m_p, respectively. The discretized time-independent single-band effective mass equation, for the pth region with constant potential energy V_p and constant effective mass m_p can be written as

$$\frac{d^2}{dz^2}\psi_p(z)+k_p^2\psi_p(z)=0 \quad \text{for } z_{p-1}\le z\le z_p \tag{2}$$

with

$$k_p=\sqrt{\frac{2m_p^*(\hat{E}-V_p)}{\hbar^2}}, \tag{3}$$

where $\psi_p(z)$ represents the envelope wave function in the pth layer, and k_p defines the complex wavevector in the same layer along z direction. The solution of Eq.(2) can be written as a superposition of a forward and a backward traveling wave functions

$$\psi_p(z)=a_p\exp(ik_pz)+b_p\exp(-ik_pz) \quad \text{for } z_{p-1}\le z\le z_p. \tag{4}$$

The boundary conditions $\psi(z)$ at the interface between layers p and (p+1) at position $z=z_p$ where p=1,2,...,(2n) are

$$\begin{cases}\psi_p(z_p)=\psi_{p+1}(z_p),\\ \dfrac{1}{m_p^*}\dfrac{d}{dz}\psi_p(z_p)=\dfrac{1}{m_{p+1}^*}\dfrac{d}{dz}\psi_{p+1}(z_p).\end{cases} \tag{5}$$

By matching the boundary conditions at each discontinuity, we arrive at

$$\begin{pmatrix}a_{2n+1}\\ b_{2n+1}\end{pmatrix}=M_{2n}\cdots M_p\cdots M_1\begin{pmatrix}a_1\\ b_1\end{pmatrix}=\begin{pmatrix}M_{11}&M_{12}\\ M_{21}&M_{22}\end{pmatrix}\begin{pmatrix}a_1\\ b_1\end{pmatrix}, \tag{6}$$

where

$$M_p=\frac{1}{2}\begin{pmatrix}\exp(-ik_{p+1}z_p)&0\\ 0&\exp(ik_{p+1}z_p)\end{pmatrix}\cdot\begin{pmatrix}1+\dfrac{k_pm_{p+1}^*}{k_{p+1}m_p^*}&1+\dfrac{k_pm_{p+1}^*}{k_{p+1}m_p^*}\\ 1+\dfrac{k_pm_{p+1}^*}{k_{p+1}m_p^*}&1+\dfrac{k_pm_{p+1}^*}{k_{p+1}m_p^*}\end{pmatrix}\cdot\begin{pmatrix}\exp(ik_pz_p)&0\\ 0&\exp(-ik_pz_p)\end{pmatrix}. \tag{7}$$

Using Eq.(6) with a_1=1, $b_1=R$, $a_{2n+1}=S$, b_{2n+1}=0, the reflection and transmission amplitudes can be obtained by

$$\begin{cases}R=-\dfrac{M_{21}}{M_{22}},\\ S=\dfrac{M_{11}\cdot M_{22}-M_{12}\cdot M_{21}}{M_{22}}.\end{cases} \tag{8}$$

The transmission coefficient $T=m_1k_{2n+1}|S|^2/(m_{2n+1}k_1)$ can be represented as a function of the longitudinal

energy, and the resonant energies can be quickly determined. We have calculated four structures, a double-barrier single-well, a three-barrier double-well, a four-barrier three-well, and a five-barrier four-well heterostructure, and the results are in excellent agreement with Ref. [10]. To get a better insight to understand the characteristics of the resonant phenomena in the open superlattices, we also solve Eq.(6) but this time with a_1=0, b_1=R, a_{2n+1}=S, b_{2n+1}=0, to yield the dispersion equation $M_{22}(\hat{E})$=0. The eigen-energies of the quasistationary states can be determined by solving the dispersion equation whose zeros are extracted numerically in the complex plane via Newton's method.

3 Results and discussion

The eigen-energies and lifetimes of a double-barrier single-well and a three-barrier double-well heterostructure are listed in Table I, compared with the APM approach (Ref. [15]) in excellent agreement. All the wave functions of the quasistationary states are adjusted to have the same amplitude $|R|$, the wave function amplitude of the right- and left-hand contacts. The relative probability density distributions in which each subband has the same coupling strength with outside contacts can be obtained. The relative probability density distributions of lower and up well subbands in a three-barrier double-well heterostructure are shown in Fig. 2. The relative probability density, $|\psi|^2$, of the lower well subbands, E_1 and E_2, are centralized about the well center, but the ones of the up well subbands, E_3 and E_4, are decentralized. The relative probabilities, the areas of the relative density probability distributions, of the lower well subbands are apparently much larger than that of the corresponding up well subbands, so the lifetimes of the lower well subbands are much larger than that of

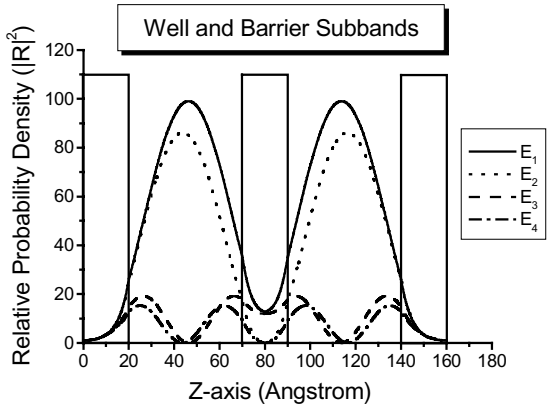

Figure 2 Relative probability density distributions of well and barrier subbands in the three-barrier double-well superlattices.

TableI. Calculation of the eigen-energies and lifetimes of the bound and quasibound states of a double-barrier single-well and a three-barrier double-well heterostructure, comparing with the APM approach in excellent agreement.

Double-Barrier Case				
Energy Level #	Quasistationary States (NM) E(meV)	τ (psec)	Quasistationary States (APM) E(meV)	τ (psec)
E_1	93.8665	0.254212	93.9	0.254
E_2	376.7840	0.024502	376.8	0.024
Three-Barrier Case				
Energy Level #	Quasistationary States (NM) E(meV)	τ (psec)	Quasistationary States (APM) E(meV)	τ (psec)
E_1	87.9702	0.581543	87.9	0.581
E_2	100.4360	0.441723	100.4	0.442
E_3	351.4360	0.058833	351.4	0.059
E_4	407.2350	0.039658	407.2	0.039

the up well subbands, respectively, as shown in Table I. One can further judge that the lifetime of the lower well subband, E_1, is larger than that of E_2, and the lifetime of the up well subband, E_3, is larger than that of E_4. Figure 3 shows the relative probability density distributions of lower well subbands in the five-barrier four-well heterostructure, and Figure 4 shows that of up well subbands. Similarly, the relative probability density of the lower well subbands, E_1, E_2, E_3 and E_4, are centralized about the well center, but that of the up well subbands, E_5, E_6, E_7 and E_8, are decentralized. The lower well subbands corresponding to the well-centralized probability density are more stable than the up well subbands corresponding to the well-decentralized probability density. From the probability density distributions, one can realize that the lifetimes of the lower well subbands, E_1 and E_4, are much larger than that of E_2 and E_3, and the lifetimes of the up well subbands, E_5 and E_8, are much larger than that of E_6 and E_7. Even small differences can be distinguished.

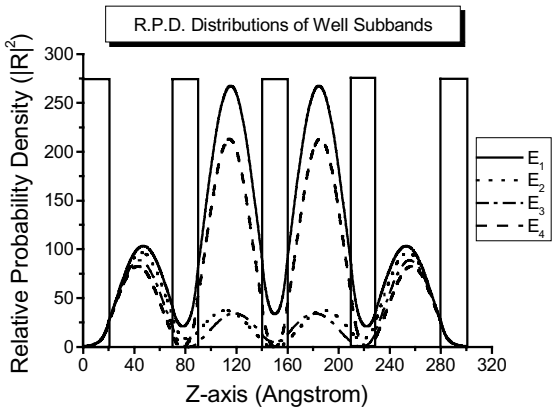

Figure 3 Relative probability density distributions of well subbands in the five-barrier four-well superlattices.

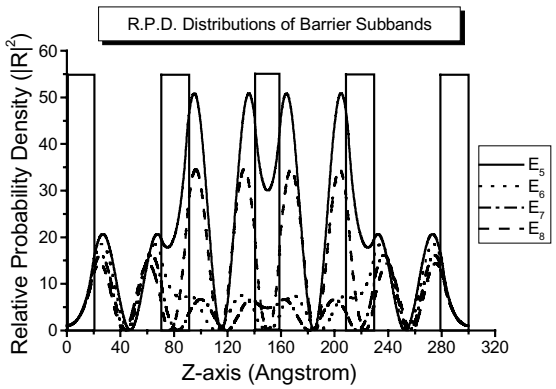

Figure 4 Relative probability density distributions of barrier subbands in the five-barrier four-well superlattices.

The lifetime of the lower well subband, E_1, is larger than that of E_4, and $\tau(E_2) > \tau(E_3)$. The lifetime of the up well subband, E_5, is larger than that of E_8, and $\tau(E_6) > \tau(E_7)$. So, the differences in lifetime between the quasibound states in the open superlattices can be easily realized with the relative probability density distributions.

4 Conclusion

In this study, we have presented a complex eigen-energy method to investigate lifetimes of the quasistationary states in superlattices, using the transfer matrix approach to discretize the conduction-band profile of the heterostructure and form a dispersion equation whose zeros correspond to the complex eigen-energies. Both the energy levels and the corresponding lifetimes are extracted numerically in the complex plane via Newton's method. The method has been proved numerically efficient and accurate by comparing with some results of the APM approach. All the wave functions of the quasistationary states have been specially adjusted to form the relative probability density distributions. With the relative probability density distributions, the differences in lifetime between the quasibound states in the open superlattices can be easily realized.

The author is also with Institute of Nanotechnology, National Chiao Tung University, Hsinchu, Taiwan 300, R.O.C.

References:

[1] F. Capasso, K. Mohammed, and A. Y. Cho, *IEEE J. Quantum Electron*., 22, 1986, 1853.
[2] D. S. Chemla et al., IEEE J. Quantum Electron. 24 (1988) 1664.
[3] B. F. Levine, J. Appl. Phys., 74, 1993, R1.
[4] S. Satta, Modular Series on Solid State Devices, Addison-Wesley, Reading, Mass., Vol**.** 8, 1989.
[5] T. K. Gaylord et al., Proc. IEEE, 79, 1991, 1159.
[6] P. J. Price, Superlattices Microstruct., 2, 1986, 593.
[7] L. Esaki and R. Tsu, IBM J. Res. Dev., 14, 1970, 61.
[8] R. F. Kazarinov and R. A. Suris, Sov. Phys. Semicond., 5, 1971, 707.
[9] R. F. Kazarinov, Sov. Phys. Semicond., 6, 1972, 120.
[10] R. Tsu and L. Esaki, Appl. Phys. Lett., 22, 1973, 562.
[11] L. Esaki and L. L. Chang, Appl. Phys. Lett., 24, 1974, 593.
[12] L. L. Chang, L. Esaki, and R. Tsu, Phys. Rev. Lett., 33, 1974, 495.
[13] J. Zamastil, J. ížek, and L. Skála, Phys. Rev. Lett., 84, 2000, 5683.
[14] K. S. Chan and R. Q. Zhang, IEEE J. Quantum Electron., 34, 1998, 2179.
[15] E. Anemogiannis, E. N. Glytsis, and T. K. Gaylord, IEEE J. Quantum Electron., 29, 1993, 2731.
[16] E. Anemogiannis, E. N. Glytsis, and T. K. Gaylord, IEEE J. Quantum Electron., 33, 1997, 742.
[17] E. Anemogiannis, E. N. Glytsis, and T. K. Gaylord, Superlattices Microstruct., 22, 1997, 481.
[18] W. Trzeciakowski and M. Gurioli, Phys. Rev. B, 44, 1991, 3880.
[19] M. Ritze, N. J. M. Horing, and R. Enderlein, Phys. Rev. B, 47, 1993, 10437.
[20] E. Anemogiannis, E. N. Glytsis, and T. K. Gaylord, Microelectronics J., 30, 1999, 935.