Dynamic Behavior and Inter-Subband Electro-Absorption of Double Quantum Wells

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Dynamic behavior of charge density and inter-subband electro-absorption spectra (including bound-to-bound and bound-to-continuum transitions) of double quantum wells under a uniform electric field is studied by a stabilization method. The double wells considered consist of one wide and one narrow well. The role of the narrow well is to provide an interference effect on the continuum states and to allow population switching. Both of these effects can significantly change the electro-absorption spectrum, thus making the double quantum well system a good candidate for an electro-optical switching device. Our study on the dynamic behavior of the coherent tunneling between two wells can also find applications in tera-hertz oscillators.

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I. Introduction

Double quantum wells (DQWs) [1-16] have attracted a great deal of interest recently because of their potential applications as opto-electronic devices (e.g., photo-detectors [1, 5], electro-optical switches [6], and tera-hertz oscillators [7, 8]) and for the study of exciton condensation [9-13]. For application in quantum well infra-red photo-detectors (QWIPs), it is important to understand the electron tunneling rate (which is related to the dark current) and the inter-subband electro-absorption spectrum (including bound-to-continuum transitions), which is related to the photo-current [1]. To the best of our knowledge, detailed theoretical calculations on inter-subband (including bound-to-continuum transitions) electro-absorption spectra for DQWs have never been reported. The tunneling rate of DQWs was discussed by Pandey and George [14] with the phase shift method, while the dynamic behavior was studied by Juang [15] and by Cruz and Muga [16] via solving the time dependent Schrodinger equation. Both methods are convenient for simple systems where the analytic solution to the wave functions is available, but become difficult to use for inhomogeneous systems with low symmetry.

In this paper, we present theoretical studies of the dynamic behavior and the inter-subband electro-absorption of DQWs via a stabilization method (SM) [17, 18] and we show that the results are significantly different from those for single quantum well (SQW) systems. For comparison purposes, we also discuss the dynamic behavior and inter-subband electro-absorption of SQW systems, which have been studied by us via analytic methods [19, 20].
In a previous paper, we showed that the tunneling rate of SQW and single quantum dot [21] can be reliably calculated via the stabilization method (SM). In SM, the local density of states (as a function of energy) of the quantum confined system is calculated and it is fitted by a Lorentzian function. The electron tunneling time is then related to the inverse of the width of the Lorentzian profile. The electron tunneling rate of SQW obtained via SM is found in excellent agreement with that obtained via the phase shift method [21]. However, at high fields we found that the local density of states is no longer well fitted by a Lorentzian function, and it is necessary to directly calculate the charge density confined in the well as a function of time (i.e., the dynamic behavior). We show in this paper that accurate dynamic behavior can also be calculated via SM. In addition, the behavior of coherent tunneling between wells which displays tera-hertz oscillations [7, 8] can be understood through the study of dynamic behavior of DQWs.

Optical absorption of uncoupled quantum wells under an electric field shows an interesting oscillatory behavior [22], which have been theoretically studied by Thzeciakowski and Gurioli [23] and by the present authors via different methods [20]. Here, we show that the stabilization method can be conveniently applied to the calculation of inter-subband electro-absorption spectra (including bound and continuum states) of both SQWs and DQWs. We found that the electro-absorption spectrum changes dramatically as the second (narrow) well is introduced due to the interference effect on the density of states. In particular, the main absorption peak is substantially narrowed and the oscillatory behavior also becomes quite different.

II. Dynamic behavior

In this section, we calculate the dynamic behavior of electrons in SQWs and DQWs via the stabilization method. We assume that initially electrons are in the ground state of the system without the applied field \( F \) and we denote the initial-state wave function by \( \hat{A}(r;0) \). The time dependent wave function of system with the applied field is turned on at \( t = 0 \) and it is written as

\[
\hat{A}(r;t) = \int dE N(E) a(E) \hat{A}(E) \exp\left\{ i \frac{E}{\hbar} t \right\},
\]

where \( N(E) \) is density of states (DOS) and \( \hat{A}(r;E) \) is the energy eigen-state of the system in the presence of the field, \( a(E) = \langle \hat{A}(E)|\hat{A}(0)| \rangle \) is the probability amplitude of finding the initial state in a given eigen-state \( \hat{A}(E) \) with energy \( E \). In Eq. (1) energies are continuous, because in the presence of the electric field, there exist no bound states, but just quasi-bound states. Although one can perform an accurate numerical integration over \( E \) using Eq. (1) to obtain the “exact” time-dependent solution as did in Ref. [19] for SQWs, it is much more convenient to obtain essentially the same result via the stabilization method (SM).

In SM [17, 18], the system is placed in a confining box with infinite barrier and length \( L \) (the scaling parameter). By performing an average over the scaling parameter \( L \), one can reproduce the results for an infinite system, as long as the physical quantity of interest depends only on the local electronic properties near the quantum well. With the introduction of the confining box, the energy levels of the system become quantized, and they are labeled by \( E_j(L) \). The density of states \( N(E) \) can be replaced by
\[ N(E) = \frac{1}{L} \sum_{j} \int_{L_0}^{L_0 + \epsilon L} \Delta(E_j(E)) \exp i \frac{E_j(L)}{E_j(L)} \]  

Equation (2) contains two contributions: one from the quasi-bound states and the other from the continuum states. The latter is proportional to \( 1 = L^2 \), while the former is insensitive to the scaling parameter \( L \), since the quasi-bound states are localized in the quantum well. In the low field limit, the lifetime of the quasi-bound state is long, and its contribution to DOS can be approximated by a Lorentzian function with a width that is directly related to the tunneling rate of the electron. At high fields, the DOS due to quasi-bound states deviates from the Lorentzian shape, and it is no longer suitable to describe the tunneling process by an exponential decay. In this case, it is better to directly calculate the time dependent wave function. Substituting Eq. (2) into Eq. (1), we obtain

\[ \tilde{\Delta}(r; t) = \frac{1}{L} \sum_{j} \int_{L_0}^{L_0 + \epsilon L} \Delta(E_j(L)) \tilde{\Delta}(r; E_j(L)) \exp i \frac{E_j(L)}{E_j(L)} \]  

The integration over energy in Eq. (1) is now replaced by an average over the scaling parameter \( L \) and a summation over the discrete index \( j \) for all quantized levels due to the large confining box. This substitution has the following advantages. In Eq. (1), the energy eigen-function \( \tilde{\Delta}(r; E) \) must be evaluated accurately with a proper normalization as a continuous function of \( E \). This can be achieved by solving the Schrödinger equation analytically as did in Ref. [19]. However, for more general cases (e.g. non-uniform potential profile as in a doped quantum well), analytic solutions are not feasible. Furthermore, the integration over \( E \) is difficult to evaluate accurately due to the fast oscillatory nature of \( \Delta(E) \) in Eq. (1). Thus, a large number of mesh points in \( E \) is needed to achieve the desired accuracy. In Eq. (3), however, all we need is to find the quantized energy levels \( E_j(L) \) and eigen-function \( \tilde{\Delta}(r; E_j(L)) \) as functions of the scaling parameter \( L \). This can be achieved by the Rayleigh-Ritz variational method which involves diagonalizing the Hamiltonian matrix defined in a finite set of basis functions. For the present system, a convenient basis to use is the collection of eigen-functions of the confining box without the presence of the quantum wells, i.e., \( \tilde{\Delta}(z) = \sin(k_m(z + L/2)) \). Throughout the paper, the origin of \( z \) is set at the middle of the confining box.

Once the time-dependent wave function is found via Eq. (3), we evaluate the charge density confined in a local volume defined as

\[ Q(t) = \int_{-Z}^{Z} j\tilde{\Delta}(r; t)^2 dr \]  

The time dependence of \( Q(t) \) for a selected local volume describes the dynamic behavior of the charge density, from which we can determine the escape rate of the electron (to leave the quantum well) or the switching rate from one well to another in DQWs. This method can be applied to arbitrary potential profile in quantum well systems as well as other nanostructures such as quantum wires and quantum dots.

To demonstrate the validity of the procedure, we first apply it to a AlGaAs/GaAs SQW system and compare the results with a previous approach [19] which utilizes Eq. (1) and solves \( \tilde{\Delta}(r; E) \) analytically in terms of linear combinations of Airy functions. The SQW has a well width...
$L_w = 51\,\text{Å}$. The effective masses used are $m_B^w = 0.095\,m_e$ (for AlGaAs) and $m_w^w = 0.067\,m_e$ (for GaAs) and the barrier height used is $V_0 = 0.247\,\text{eV}$. The above set of parameters give two bound states for the SQW with the ground state energy $E_0 = -0.174\,\text{eV}$ and excited state energy $E_1 = -0.004\,\text{eV}$ (with respect to the top of the well).

Using 50 basis functions to diagonalize the Hamiltonian for a SQW placed in the middle of a confining box with length $L$, we obtain the eigen-values and eigen-vectors as functions of $L$. The stabilization graph ($E_j(L)$ versus $L$) for the the lowest 15 eigen-values at a field $F = 200\,\text{kV/cm}$ is shown in Fig. 1. Throughout the paper, the energy zero is set at the top of the well in the absence of the field. In Fig. 1 there is only one quasi-bound state. The original shallow bound state with energy $E = -4\,\text{meV}$ is pushed out the well into the continuum by the electric field.

Using Eq. (3) and (4), we obtain the charge density confined in the well $Q(t)$. Fig. 2 shows $Q(t)$ as a function of $t$ for different field strengths (all considered high fields). Solid curves from top to bottom are for $F = 200, 250$ and $300\,\text{kV/cm}$, respectively. Also included for comparison are the exact solutions (dotted curves) obtained via the analytic method [19]. As seen in the figure, the dynamic behavior of $Q(t)$ obtained with SM is in excellent agreement with that calculated via the analytic method. Note that $Q(0) = 0.873$, which indicates the initial charge density confined in the well with a finite potential barrier. $Q(t)$ in Fig. 2 displays an oscillatory behavior which is caused by the quantum interference between forward and backward scattered waves as the electron tunneling out the triangular potential barrier established by the conduction band offset and the electric field.

We now apply SM to the DQW system. We consider a double-well structure which consists of a left well with width $L_1 = 51$ and a right well with width $L_2 = 20$. Barrier height and barrier thickness are $V_0 = 0.247\,\text{eV}$ and $L_B = 80$, respectively. The energy of the ground state (confined in left well) is $-0.174\,\text{eV}$ and the energy of the first excited state (confined in the right well) is $-0.083\,\text{eV}$ in the absence of the field.

![Fig. 1. Stabilization graph showing the lowest 15 eigenvalues as functions of the box size $L$ for a AlGaAs/GaAs SQW with well width 51 Å and applied field $F = 200\,\text{kV/cm}$.](image1)

![Fig. 2. Charge density $Q(t)$ of a AlGaAs/GaAs SQW with well width 51 Å for different fields. Solid curves (from top to bottom) denote $F = 200, 250,$ and $300\,\text{kV/cm}$, respectively. Dotted curves are obtained by an analytic method as described in Ref. [19].](image2)
FIG. 3. Charge density $Q_T(t)$ of an AlGaAs/GaAs DQW with $L_1 = 51\AA$, $L_2 = 20\AA$, and $L_B = 80\AA$ for different strengths of applied field: $F = 80$ kV/cm (dashed line), $F = 150$ kV/cm (dot-dashed line), and $F = 200$ kV/cm (solid line).

Fig. 3 shows the total charge density $Q_T(t)$ confined in both wells with $z < L_B = 2 + L_2$ ($z = 0$ corresponds to the center of the $80\AA$ wide barrier) as a function of $t$ at three different fields: $F = 80$ kV/cm (dash line), $F = 150$ kV/cm (dot-dashed line), and $F = 200$ kV/cm (solid line). Similar to the SQW case, 50 sine functions were used as the basis in this calculation. There exists a resonant field $F_r$, at which the energies of quasi-bound states confined in the left and right wells coincide, and resonant tunneling of the electron occurs. This field is around 80 kV/cm. Without the resonant tunneling effect (e.g., the SQW case), the electron escape rate would increase with increasing field as shown in Fig. 2. However, with the resonant tunneling effect, the electron can escape from the well much faster at the resonant field ($F_r$) than at other fields, even though the latter is higher than $F_r$. From Fig. 3, we see that the charge density $Q_T(t)$ at $F = 80$ kV/cm leaks out much more quickly than other two higher fields, indicating the effect of resonant tunneling. At the highest field ($F = 200$ kV/cm) there is a sudden drop of $Q_T(t)$ from 1 and fast oscillation on the small time scale ($t < 200$ fs). This behavior is similar to the SQW case, and the physical mechanism for that has been discussed in Ref. [19]. On the large time scale, the charge density $Q_T(t)$ decays exponentially at $F = 200$ kV/cm. This is expected, since at this field, the energies of quasibound states confined in the left (wide) and right (narrow) well are far separated, so there exists no beating effect between the two levels. Near the resonant field ($F = 80$ kV/cm), the energy levels of the two quasi-bound states are close enough to produce a beating effect, which results in a pronounced charge oscillation on a time scale of 1000 fs. Such a terahertz oscillation has been studied previously [7, 8]. Here, we provided a convenient method to analysis the dynamic behavior of such tera-hertz oscillators. For the intermediate field ($F = 150$ kV/cm), the time dependence of $Q_T(t)$ does not show a clear beating effect nor an exponential decaying behavior.

Fig. 4 shows the total charge density confined in both wells, $Q_T(t)$ and the charge density
confined in the right well only, $Q_R(t)$ (with $L_B = 2 < z < L_B = 2 + L_2$) as functions of $t$ for different barrier widths and for a field near the corresponding resonant field ($F_r$). We denote the energy separation of the quasi-bound states confined in the left and right well by $\xi \bar{E}$ (absolute value). Dashed lines are for $L_B = 60\text{Å}$ (with $F = 95 \text{ kV/cm}$ and $\xi \bar{E} = 4.6 \text{ meV}$), solid lines are for $L_B = 80\text{Å}$ (with $F = 80 \text{ kV/cm}$ and $\xi \bar{E} = 2.3 \text{ meV}$), and dot-dashed lines are for $L_B = 100\text{Å}$ (with $F = 70 \text{ kV/cm}$ and $\xi \bar{E} = 4.1 \text{ meV}$). The upper and lower sets of lines are for $Q_T(t)$ and $Q_R(t)$, respectively. A beating behavior is clearly visible in this figure for $L_B = 60$ and $80\text{Å}$, and the beating period is inversely proportional to $\xi \bar{E}$ as expected. Note that $Q_T(t) \perp Q_R(t)$ corresponds to the charge density confined in the left well of the DQW system. So, when $Q_T(t)$ is approximately the same as $Q_R(t)$ (see the dashed lines at $t \approx 500 \text{ fs}$), it means that the charge density switches almost completely from the left well to the right well. Thus, the estimated carrier switching time is about $500 \text{ fs}$ for the $L_B = 60\text{Å}$ DQW, and $800 \text{ fs}$ for the $L_B = 80\text{Å}$ DQW. The charge oscillation is much more pronounced in the thin barrier case (dashed lines) than the thick barrier case (solid and dot-dashed lines). For the thickest barrier ($L_B = 100\text{Å}$), $Q_R(t)$ is negligibly small at all times. However, $Q_T(t)$ still shows a long-period oscillation. Thus, we found that large barrier width suppresses the amplitude of $Q_R(t)$. Similar result was also reported by C. Juang [15].

### III. Inter-subband absorption

In this section we discuss the inter-subband electro-absorption spectra of SQWs and DQWs obtained with the stabilization method. The inter-subband absorption coefficient is given by [20],

$$
\bar{\alpha}(\omega) = \frac{1}{\sqrt{\pi} c \tau_s! m_e^2} \left(\frac{4}{3}\right) \frac{\bar{E}^2}{\pi} \epsilon \mathcal{N}(\bar{E}) M_{\bar{E},\bar{E}}^2 \sum_{\bar{E}} \left(\frac{\bar{E}}{\bar{E}}\right)^2 \left(\frac{\bar{E}}{\bar{E}}\right)^2 \epsilon \mathcal{N}(\bar{E}) \right)
$$

where $\omega$ is the energy of incident photon, $E_i(E_f)$ is the energy of the initial (final) state, $f(E)$ is the Fermi-Dirac distribution function, $V$ is the volume of the active region, $\tau_s$ is the refractive index, and $c$ is the speed of light. $M_{\bar{E},\bar{E}}$ is the optical matrix element for an incident photon polarized in the $z$ direction,

$$
M_{\bar{E},\bar{E}} = \sum_{\bar{E}} \int_{-\infty}^{\infty} \frac{d\epsilon}{\pi} \sum_{\bar{E}} \epsilon \mathcal{N}(\bar{E}) \epsilon \mathcal{N}(\bar{E}) \left(\frac{\bar{E}}{\bar{E}}\right)^2 \left(\frac{\bar{E}}{\bar{E}}\right)^2 \epsilon \mathcal{N}(\bar{E}) \right)
$$

where $\bar{A}_i(z)$ and $u_{E_i}(z)$ are the initial and final state wave functions, respectively. $p = i$ $i$ $r$ is the momentum operator. We approximate the initial-state wave function $\bar{A}_i(z)$ by the ground state eigen-function of the system with $F = 0$ and use the equilibrium carrier distribution as determined at $F = 0$. These approximations are good as long as $V_0 \bar{A} \left(\epsilon eF\right)^2 \approx m_B^{1/3}$ [24]. To apply SM to the problem, we substitute the density of states $\mathcal{N}(\bar{E})$ in Eq. (5) by the expression given in Eq. (2) and obtain

$$
\bar{\alpha}(\omega) = \frac{1}{\sqrt{\pi} c \tau_s! m_e^2} \left(\frac{4}{3}\right) \frac{\bar{E}^2}{\pi} \epsilon \mathcal{N}(\bar{E}) M_{\bar{E},\bar{E}}^2 \sum_{\bar{E}} \left(\frac{\bar{E}}{\bar{E}}\right)^2 \left(\frac{\bar{E}}{\bar{E}}\right)^2 \epsilon \mathcal{N}(\bar{E}) \right)
$$
FIG. 5. Stabilization graph showing the lowest 15 eigenvalues as functions of the box size $L$ for a AlGaAs/GaAs SQW with well width 51 Å and applied field $F = 70$ kV/cm.

Here we again consider the AlGaAs/GaAs systems, since experimental results for these systems are more readily available. First we examine the SM calculation for a Al$_{0.3}$Ga$_{0.7}$As/GaAs SQW system, which was also studied previously by us via an analytic method [20]. All parameters used here are the same as those in last section.

Fig. 5 shows the stabilization graph (SG) of the SQW at $F = 70$ kV/cm. It is noted that a stable horizontal line appears at $E = 0.1749$ eV, which is corresponding to the quasi-bound state. A small red Stark shift of 0.9 meV is found. The second bound state at $F = 0$ has become unbound at this field. The oscillatory parts of the curves in this figure represent the anti-crossing pattern of the resonance states interacting with the continuum states which lead to oscillatory features in the absorption spectrum shown below.

Using Eq. (7) we calculate the zero-temperature inter-subband absorption spectra of the SQW system at finite fields. Only $k_F = 0$ ($k_F$ is the in-plane wave vector) contribution is considered. The contributions due to all $k_F$ only amount to a slight broadening of the spectrum as discussed in Ref. [20]. Fig. 6 shows the inter-subband absorption spectra of the SQW system at $F = 70$ kV/cm (solid line), 100 kV/cm (dashed line), and 130 kV/cm (dot-dashed line). The main effect of the electric field is to shift the peak position of the absorption spectrum to higher energy and to cause a broader spectrum as $F$ increases. These results are in good agreement with those calculated by the analytic method reported in Ref. [20], so we have demonstrated that SM can be used to calculate inter-subband electro-absorption spectra of quantum well systems. The same method should be equally applicable to other nanostructure systems, where the analytic method is not feasible.

Next we use SM to calculate the inter-subband electro-absorption spectra of DQW systems. DQWs have some useful applications, since the electronic and optical properties are sensitive to the change in the applied field. We consider the case that the Fermi level of the system is just above the ground state level, so that only the wide well is populated at $F = 0$. The presence of the narrow well serves two purposes: one is to interfere with the continuum states in order to
modify the density of states, and the other is to cause a population switching as the field is increased. Both of these effects can substantially modify the inter-subband absorption spectrum, thus making the system suitable for application as an electro-optical switching device or a multi-colored infra-red detector.

Fig. 7 shows the stabilization graph of the DQW system with \( L_B = 80 \text{Å} \) at \( F = 70 \text{kV/cm} \). The system has two quasi-bound states with energies \( E_0 = -0.175 \text{eV} \) and \( E_1 = -0.165 \text{eV} \), which correspond to the stable horizontal lines in this figure. The former is associated with a confined level in the wide well, and the latter with a confined level in the narrow well. As seen in this figure, there is a quasi-bound state with energy slightly below zero (-0.015 eV). This level is related to the first resonance level of the SQW system which appears at \( E = 0.08 \text{eV} \) in Fig. 5. The level is pulled down due to the presence of the narrow well in the DQW which introduces a negative perturbation to the SQW system. This level is responsible for the first peak in the inter-subband absorption spectrum to be discussed below.

Fig. 8 shows the inter-subband absorption spectra of DQWs at \( F = 70 \text{kV/cm} \) for two different widths of tunneling barrier: \( L_B = 80 \) and 110 Å. They are denoted by dashed line and dot-dashed line, respectively. Also included for comparison is the SQW inter-subband absorption spectrum (solid line), which is duplicated from the solid line of Fig. 6. From this figure, we see that the absorption spectra of DQWs have much sharper peaks compared to the SQW case, indicating the strong interference effect caused by the presence of the narrow well. The first peak of the dashed line is due to the transition from the lowest quasi-bound state to the quasi-bound state with energy just below zero (the first resonance level) as mentioned above (see Fig. 7). The other peaks are associated with transitions from the lowest quasi-bound state to the higher resonance states which are also apparent in the SG (Fig. 7). For large barrier thickness \( L_B = 110 \text{Å} \) the lowest quasi-bound state becomes localized in the narrow well, since the electrical potential terms \( -eFz \) lowers the narrow well ground level much more than its effect on the wide well ground level. Thus, the carrier population switches from the wide well to the narrow well [6].
Absorption spectrum after population switching has been shown by dot-dashed line in which the first peak is corresponding to the transition between the quasi-bound state at $E = 1858 \text{ eV}$ (now localized in the narrow well) and the second resonance state at $E = 0.033 \text{ eV}$, which is also localized near the narrow well. Thus, we have demonstrated that the presence of the second (narrow) well can lead to a substantial change in the inter-subband absorption spectrum and the change is sensitive to the strength of applied field.

We have also studied the case of the reverse bias (i.e., $F < 0$). For the reversed bias, we found that the inter-subband absorption spectrum of the DQW system is almost identical to that of the SQW system. This is because the continuum states which contribute to the absorption are localized at the left side of the left well (due to reverse bias), thus experiencing no interference effects from the presence of the narrow well on the right side of the wide well. Furthermore, no charge switching occurs, since the quasi-bound level associated with the narrow well remains above the Fermi level.

For applications in electro-optical switching devices, one is interested in how the absorption spectrum can be modulated by the applied electric field, Fig. 9 shows the inter-subband absorption spectra of a AlGaAs/GaAs DQW with $L_1 = 51 \text{Å}$, $L_2 = 20 \text{Å}$, and $L_B = 80 \text{Å}$ at three different fields: $F = 55 \text{ kV/cm}$ (solid line), $70 \text{ kV/cm}$ (dashed line), and $100 \text{ kV/cm}$ (dot-dashed line). At higher field $F = 100 \text{ kV/cm}$, the carrier population is completely switched from the wide well to the narrow well. The absorption spectra for these three field are significantly different, indicating the suitability of the DQW system as an electro-optic switching device.
IV. Summary

We have studied the dynamic behavior of electron tunneling process and inter-subband electro-absorption spectra of double quantum wells (DQWs) via a stabilization method (SM). We show that SM can be conveniently used to calculate not only the tunneling rate (long time behavior and small field) [21] but also the dynamic behavior of tunneling process (short time behavior and large field). We found that at the resonant field $F_r$, the electron escape rate is substantially increased due to the resonant tunneling process. Our calculation also provides an analysis of the electron charge oscillation between the left well and the right well in the coherent tunneling process.

We also demonstrated that SM can be used to calculate the inter-subband electro-absorption spectra of single quantum well (SQW) as well as double quantum well (DQW) systems. The results so obtained for SQW system are in agreement with those obtained by an analytic method for an infinite system, thus establishing the validity of the method. The inter-subband absorption spectra of DQWs are found to be sensitive to the thickness of the spacer barrier between the two quantum wells and the strength of the electric field. Our studies provide a detailed analysis of the DQW systems which have useful applications in tera-hertz oscillators, electro-optical switching devices, and multi-colored infra-red detectors.

References