Possiblity of terahertz emission with a time-dependent amplitude in semiconductor quantum wells

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In this work, we have numerically integrated in space and time the effective-mass Schrödinger equation for an exciton in a semiconductor structure. Considering a Coulomb interaction between the electron-hole pair in a triple quantum-well system, we have obtained a time-varying dipole moment in the heterostructure with an amplitude which is also oscillating with time. In this way, we have shown the possibility of having another kind of terahertz electromagnetic radiation emerging from a semiconductor device after an optical excitation of the sample.

Since its discovery by Tsu and Esaki,[1] tunneling in semiconductor quantum wells has been the object of great attention. In the last years, quantum wells have shown many interesting optical and electronic properties[2] playing a key role in many electronic devices such as field-effect transistors, photodetectors, and quantum-well lasers.[2,3] Recently, $GaAs/Ga_xAl_{1-x}As$ semiconductor coupled quantum wells have been used to observe tunneling charge oscillation in solids.[4] In such an experiment, the superposition of both symmetric and antisymmetric quantum-well eigenstates in the conduction band lead to coherent tunneling between both quantum wells, and thus, to an electron-hole pair with a time-dependent distance. In this way, a time-varying excitonic dipole moment was obtained in the wells that allowed the emission of electromagnetic radiation at the oscillation frequency. Among the different semiconductor structures studied in the past, coupled quantum wells present the appealing feature of having terahertz emission emerging from the sample after optical excitation. Thus, considerable attention to these structures can be expected due to their possible applications as ultrahigh-frequency optoelectronic emitters.

In view of such recent experiments[4,5] involving time-dependent excitonic processes in single and double quantum wells, there is an urgent need to examine the dynamical evolution of the excitonic electron-hole pairs, not only the stationary aspects.[6] Taking this into account, in this work we will study the time-dependent evolution of electron-hole pairs in a semiconductor structure considering a Coulomb interaction between both carriers. The method of calculation will be based on the discretization of space and time for the carrier wave functions. To have a dynamical evolution for both carrier wave packets, in our calculations we will consider a triple quantum-well potential (Fig. 1). In Fig. 1, we have plotted a schematic picture of a triple quantum-well structure. The left well, center well, and right well consist of GaAs, while the barrier between the wells consists of $Ga_{1-x}Al_xAs$. When no electric field is applied [Fig. 1(a)], the electron and hole states are predominantly localized in their respective wells. Application of F_r electric field causes quantum-mechanical resonance accompanied by a delocalization of the electron wave functions over the center and right wells in the conduction band [Fig. 1(b)]. Note that, in principle, hole levels should be out of resonance at F_r. However, in our coupled quantum-well system, we have chosen a wide left well that also allows coherent tunneling between the left and center well in the valence band at F_r. In addition to this, the coupled quantum system of Fig. 1(b) provides the possibility to discriminate optical transitions in the three wells by their different spectral positions. In this way, resonant optical excitation of the center well will create both electron and hole wave packets localized initially in the center well. Both packets are linear superposition of the two eigenstates in the conduction and valence bands, and hence, nonstationary. Subsequently, the electron packet will oscillate between the center and right wells and the hole packet between the center and left wells with two different periods. In addition to these electron and hole charge oscillations, there is an excitonic Coulomb interaction between both carriers that will be also considered in our method of calculation. Finally, we will show that the dynamics of a photoexcited electron-hole pair in the center well at $F=F_r$ will allow the existence of a new kind of time-dependent dipole moment in the system, and thus, a new kind of terahertz emission emerging from the device.

In order to study the dynamics of tunneling, we need to solve the time-dependent Schrödinger equation associated with the Hamiltonian for a spinless exciton in the heterostructure region. The excitonic wave function Φ is

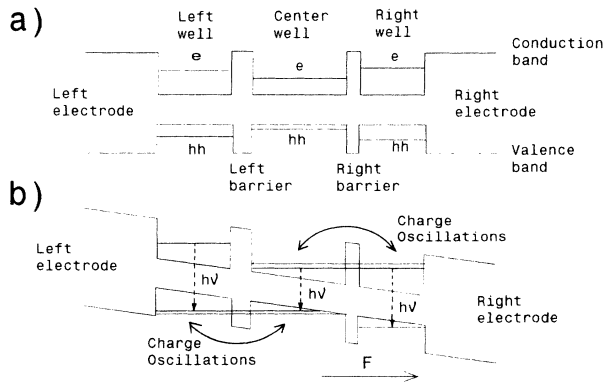

FIG. 1. (a) Triple quantum-well system in absence of external applied electric field. (b) The heterostructure potential at the resonant condition for both conduction and valence bands.

given by

$$\left[-\frac{\hbar^2}{2\mu_{xy}}\nabla_{xy}^2+\sum_{i=e,h}\left[-\frac{\hbar^2}{2m_i^*}\frac{\partial^2}{\partial z_i^2}+V_i(z_i)\right]+V_C(\rho,z_e-z_h)\right]\Phi(\mathbf{r}_e,\mathbf{r}_h)=i\hbar\frac{\partial}{\partial t}\Phi(\mathbf{r}_e,\mathbf{r}_h)\ , \quad (1)$$

where the subscripts e,h refer to electrons or holes, respectively, and $V_e(z_e)$, $V_h(z_h)$ are the potentials due to the quantum wells. The m_e^* and M_h^* values are the effective masses, μ_{xy} is the reduced x-y plane electron-hole mass, and $\rho=\rho_e-\rho_h$ is the relative motion within the quantum-well plane. Neglecting the difference in the dielectric constants for well and barrier, the Coulomb potential is

$$V_C(\rho,z_e-z_h)=-\frac{e^2}{\epsilon\sqrt{\rho^2+(z_e-z_h)^2}} \quad (2)$$

and now we separate the total wave function Φ into the motion along z and the in-plane motion of the exciton $\phi(\rho)$,

$$\Phi=\Psi(z_e,z_h)\phi(\rho) \quad (3)$$

persisting Coulomb effects in the growth direction

$$\left\{\sum_{i=e,h}\left[-\frac{\hbar^2}{2m_i^*}\frac{\partial^2}{\partial z_i^2}+V_i(z_i)\right]+W(z_e-z_h)\right\}\Psi(z_e,z_h)=i\hbar\frac{\partial}{\partial t}\Psi(z_e,z_h)\ , \quad (4)$$

as the potential

$$W(z)=\int_0^\infty d\rho\,\rho\left[\frac{\hbar}{2\mu_{xy}}[\partial_\rho\phi(\rho)]^2-\frac{e^2}{\epsilon\sqrt{\rho^2+z^2}}\phi^2(\rho)\right] \quad (5)$$

has to be added to the heterostructure potentials.[7] This two-variable Schrödinger equation can be simplified introducing the factorization $\Psi(z_e,z_h)=\psi(z_e)\psi(z_h)$, and thus, obtaining the equations,

$$\left[-\frac{\hbar^2}{2m_e^*}\frac{\partial^2}{\partial z_e^2}+V_e(z_e)+W_h(z_e)\right]\psi_e(z_e)=i\hbar\frac{\partial}{\partial t}\psi_e(z_e)\ , \quad (6)$$

$$\left[-\frac{\hbar^2}{2m_h^*}\frac{\partial^2}{\partial z_h^2}+V_h(z_h)+W(z_h)\right]\psi_h(z_h)=i\hbar\frac{\partial}{\partial t}\psi_h(z_h)\ , \quad (7)$$

that have to be solved together since the term

$$W_i(z)=\int dz'\psi_i^2(z')W(z-z') \quad (8)$$

couples ψ_e and ψ_h being $I=e,h$. To simplify our calculation we have used for the in-plane motion of the exciton the ansatz[8]

$$\phi(\rho)=\frac{2}{a}e^{-\rho/a}\ , \quad (9)$$

where a is the two-dimensional excitonic radius.

Let us discretize time by a superscript n and spatial position by a subscript j and k for the conduction and valence band, respectively. Thus, $\psi_e\rightarrow\kappa_j^n$ and $\psi_h\rightarrow\varphi_k^n$. The various $z_{e,h}$ values become $j\delta z$ and $k\delta z$ in the conduction and valence band, where δz is the mesh width. We have taken the same δz value for the conduction and valence band. Similarly, the time variable takes the values $n\delta t$, where δt is the time step. The second-order spatial derivative is approximated as

$$\kappa_j''=\frac{1}{\delta z^2}(\kappa_{j+1}-2\kappa_j+\kappa_{j-1})+O(\delta z^2) \quad (10)$$

in the conduction band and

$$\varphi_k''=\frac{1}{\delta z^2}(\varphi_{k+1}-2\varphi_k+\varphi_{k-1})+O(\delta z^2) \quad (11)$$

in the valence band. To treat the time development we have used a unitary propagation scheme for the evolution operator in both conduction and valence bands,[9]

$$\kappa_j^{n+1}\varphi_k^{n+1}=\frac{1-iH\delta t/2}{1+iH\delta t/2}\kappa_j^n\varphi_k^n \quad (12)$$

obtaining a tridiagonal linear system that is solved by standard numerical methods.[9] In our calculations, we have assumed that an electron-hole pair is initially created in the center quantum well at $t=0$. Then, Eqs. (6) and (7) are numerically solved using spatial mesh size of 0.5 Å, a time mesh size of 1 fs, and a finite box (2000 Å) large enough as to neglect border effects. In our calculations, we have considered a triple-well GaAs/$Ga_{0.25}Al_{0.75}As$ semiconductor system which consists of a 73-Å-wide left quantum well, a left barrier of 40 Å thickness, a 50-Å-wide center, a right barrier of 25 Å thickness, and a 100-Å-wide right quantum well, Fig. 1(a). We have assumed a $m_e^*=0.067m_0$ effective mass in the conduction band and a $m_h^*=0.7m_0$ heavy-hole mass. We have used a valence-band offset of 0.138 eV obtaining small values for the barrier height in the valence band. With such a triple quantum-well system, the electron energy levels of the right and center wells are aligned in the conduction band at $F_r=38.6$ kV/cm, while in the valence band both hole levels in the left and center wells are aligned at the same electric field, Fig. 1(b). This effect is allowed by our structure-potential parameters. In this way, the electron and hole charge density will oscillate in both bands with a certain tunneling period at F_r. We have neglected the mixing effects in the valence band. Such an approximation is well justified for our structure's potentials.[6]

Neglecting the Coulomb interaction between the electron-hole pair, the excitonic dynamics will be basically determined by means of two different coherent tunneling processes in both bands. In the system, the electron and hole wave packets will oscillate with two different periods due to the different carrier effective masses. From a semiclassical point of view, such a period τ can be estimated as follows:[10]

$$\tau=\lambda\,dm^*\exp(2\pi d/\lambda)\ , \quad (13)$$

where $\lambda=h/\sqrt{2m^*(V_0-E)}$ is the de Broglie wave-

length of the tunneling carrier and V_0 the barrier height.

The numerical integration in time allows us to obtain the electron and hole charge density $Q^{e,b}$ in a defined semiconductor region $[a,b]$ at any time t,

$$Q_{ab}^{e,h}(t)=\int_a^b dz_{e,h}|\psi^{e,h}(z_{e,h},t)|^2 . \quad (14)$$

In Fig. 2, we have plotted $Q_{ab}^{e,h}$ versus time, a and b being the center quantum-well limits. It clearly shows the existence of carrier charge-density oscillations for both electron and hole packets placed in the center well at $t=0$. The oscillation period can be easily determined by analyzing the position of the charge-density peaks in the curves. In order to compare our numerical results with the estimated oscillation period values of Eq. (13), we have included two barriers of infinite height in both device electrodes. In this way, we neglect the field-induced escape tunneling process of electrons and holes to the right and left electrode, respectively, obtaining precise results for the oscillation periods. Later, we will estimate the role of the escape tunneling processes in the device. In principle, we have found that the numerical results plotted in Fig. 2 are in reasonable agreement with Eq. (13), if we change m^* by the electron or hole mass. Thus, the Coulomb interaction between the excitonic pair can be considered as a correction term in the total Hamiltonian. With or without the electron-hole interaction, the differences in the calculated tunneling times are about 10–20%. A similar result was obtained by Mohaidat, Shum, and Alfano[11] in the study of single-electron tunneling in asymmetric quantum wells. Varying the left barrier thickness d in the triple quantum well, we have obtained an increase in the hole period value τ_h. The resonant condition F_r slightly varies in each case. This result can be easily explained taking into account Eq. (13). Defining the ratio between both carrier periods as

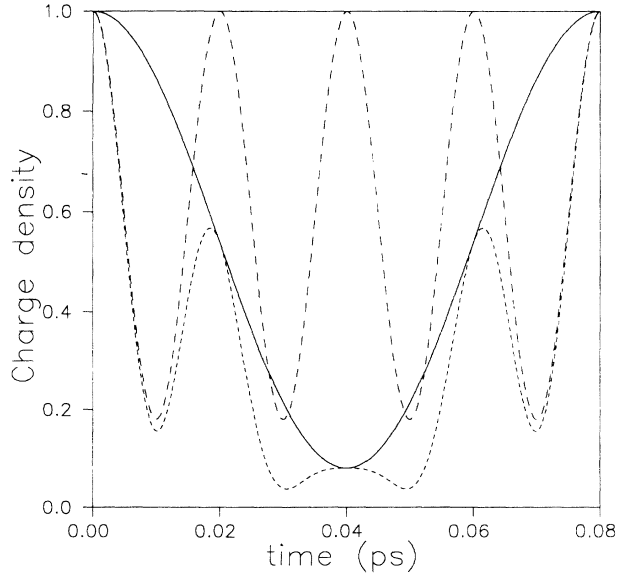

FIG. 2. Carrier charge density vs time [Eq. (14)]. Long-dashed line, electron charge density. Solid line, hole charge density. Short-dashed line, excitonic charge density that is the product of the electron and hole densities.

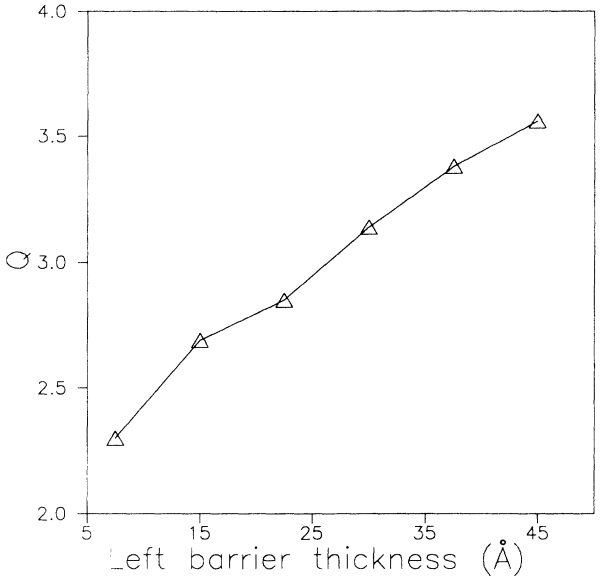

FIG. 3. The ratio between the hole and the electron tunneling period (Q) vs the left barrier thickness (d).

$Q=\tau_e/\tau_h$, we have plotted Q versus d in Fig. 3. We should note that Q represents the number of electron peaks that are in each large-period oscillation (Fig. 2). So that, in the time that the hole makes a single oscillation between the center and left wells, Q determines the number of electron oscillations between the center and right wells. In this way, we have an oscillating electron-hole distance, with the conduction-band frequency, with its amplitude also oscillating with the valence-band tunneling period. We have also shown in Fig. 3 that we can determine both oscillation frequencies through the sample characteristics. We can expect that such an excitonic pair will emit electromagnetic radiation at the dipole fre-

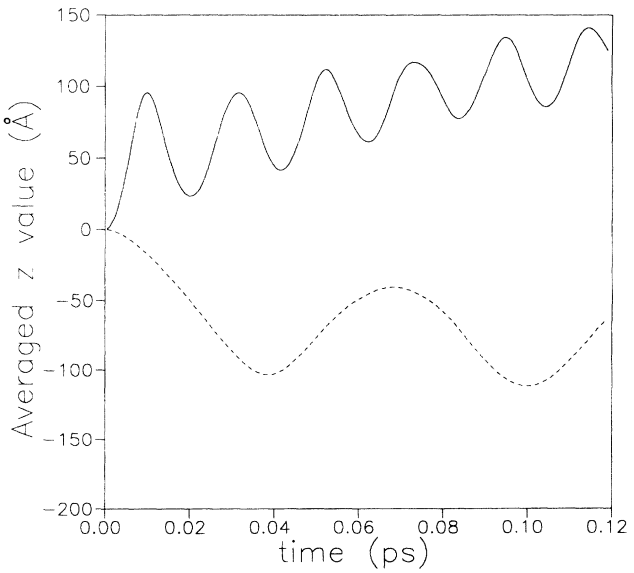

FIG. 4. Solid line, the averaged z value of the electron charge density vs time. Dashed line, the averaged z value of the hole charge density vs time.

quency given its amplitude also oscillating with time.

In Fig. 4, we have plotted the average value of electron and hole charge density at different times. It is clearly shown that the electron position is oscillating between the center and left well while the hole position is doing that between the center and right well. In addition to the electron position oscillation in Fig. 4, it is also found that its averaged value increases with time. We can easily explain such an effect taking into account the tunneling escape process of the electron charge density to the right electrode in the device. However, in the valence band we note that the field-induced hole tunneling process to the left electrode is not significantly important. The differences between both escape tunneling processes can be explained taking into account the higher effective-mass value in the valence band. Such an effect is not very important for small t values but it should be taken into account in the case of an experimental observation at large t. For example, in Ref. 5 Planken *et al.* obtained experimental measurements for fourteen electron charge oscillations on two coupled quantum wells in the conduction band.

In summary, in this work we have numerically integrated in space and time the effective-mass Schrödinger equation for an electron-hole pair in a quantum-well structure. We have obtained that the excitonic dynamics is basically determined by two different oscillation periods that are related with the existence of coherent tunneling processes in both conduction and valence bands. It is also found that the ratio between both period values can be determined through the sample characteristics. Taking into account that the mean life for an electron-hole pair in GaAs is 200 ps, in principle, an experimental observation of such a process is possible. In this way, we have shown the possibility of having a different kind of electromagnetic emission emerging from a semiconductor triple quantum-well system after an optical excitation of the sample.

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