STARK RESONANCE PROPERTIES IN SEMICONDUCTOR QUANTUM WELLS UNDER STRONG TRANSVERSE ELECTRIC FIELDS: A REAL-TIME OPTICAL-POTENTIAL WAVEPACKET PROPAGATION METHOD

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ABSTRACT

The energies, lineshapes, lifetimes, and eigenfunctions of all the Stark resonances arising in GaAs-(Ga,Al)As quantum wells with widths ranging from 50 Å to 200 Å, under transverse electric fields with strengths from 300 kV/cm to 1000 kV/cm are reported, for both electrons and holes. The constant-effective-mass and single-hole-band approximations are employed, and the (unimportant at high fields) electron-hole interaction is neglected. The Real-Time Wavepacket Propagation Method was implemented for this task, together with an asymptotic (absorbing) optical potential, which allows the simulation of the continuum with a finite computational grid and the filtering of the non-resonant part out of the test function. This approach yields all the resonance properties of a given structure in a single calculation.

INTRODUCTION

When a quantum system is subjected to a dc field, the formerly discrete quantum states become metastable (tunnelling resonances) and their energies are shifted. In semiconductor heterostructures this phenomenon is known as the **q**uantum-**c**onfined **S**tark **e**ffect (QCSE), which is important from both the fundamental[1] and the optoelectronics[2] standpoints. In strong fields and/or for excited states, it is necessary to consider the field-induced tunnelling besides the field-induced (Stark) shift[3].

The problem of the QCSE has been addressed using *ab initio* pseudopotential,[4] variational,[5] Airy functions with complex[6,7] and real[8] arguments, transfer matrix,[8,9] finite difference,[10,11] finite element,[12] complex coordinate,[13] stabilization-graph,[14] and Fourier series[14] methods. The advantages of time-dependent methods[10-14] over time-independent ones[4-9] for tunnelling problems have been widely discussed in the literature[10,14-16].

In this work, the positions, lineshapes, lifetimes, and eigenfunctions of all the Stark resonances arising in GaAs-(Ga,Al)As quantum wells (QWs) under strong transverse electric fields are determined, for both electrons and holes. The constant effective-mass and single-hole-band approximations are employed, and the (unimportant at high fields) electron-hole interaction is neglected. The Real-Time Wavepacket Propagation Method (RTWPM), implemented earlier for discrete[17,18] and continuous[17] spectra, is supplemented with a smooth optical (absorbing) potential,[19] in order to filter the (uninteresting) non-resonant part out of the test function[15] and to simulate the continuum, at the same time employing a finite computational grid.[15,17,19,20] This

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approach shares the advantages of other time-dependent numerical methods[10-14] (accuracy, flexibility, and automatic enforcement of boundary conditions), with the additional advantage of yielding the entire eigenspectrum, including the lineshape, of a given structure in a single calculation.

Results are reported for QWs with widths ranging from 50 Å to 200 Å and field strengths from 300 kV/cm to 1000 kV/cm, where strong field-induced resonance features are observed.

FORMALISM

Resonances. In this paper, for *interpretation* purposes, a resonance appearing in the continuous spectrum of a system with hamiltonian $\hat{H}$ is modeled as a discrete, L^2, complex eigenstate[15,21] of an associated, non-hermitian hamiltonian $\hat{\tilde{H}}$,[22] $\hat{\tilde{H}}\varphi_n(q) = E_n\varphi_n(q)$. Here q denotes the full set of generalized coordinates, and

$$E_n = \varepsilon_n - i\Gamma_n/2 \qquad [1]$$

is the corresponding complex eigenenergy, with ε_n the energy at the resonance peak. The associated "stationary" state takes the form

$$\Phi_n(q,t) = \varphi_n(q)\exp[-i(\varepsilon_n - i\Gamma_n/2)t/\hbar], \qquad [2]$$

whose norm $< \Phi_n(t) \mid \Phi_n(t) >= \exp(-\Gamma_n t/\hbar)$ is seen to decay in time with a lifetime

$$\tau_n = \hbar/\Gamma_n . \qquad [3]$$

For *computational* purposes, the L^2 complex resonance eigenfunction is also expressed formally as a spectral expansion in terms of the (real) continuum eigenstates of the true hamiltonian $\hat{H}$:

$$\varphi_n(q) = \int c_n(\varepsilon)\psi_\varepsilon(q)d\varepsilon, \qquad [4]$$

where ε labels the continuous energy variable. The evaluation and comparison of the spectral functions[17,18] associated with (2) and (4) indicate that the relative spectral weights of the continuum states contributing to the resonance are given by

$$|c_n(\varepsilon)|^2 = \mathrm{L}(\varepsilon - \varepsilon_n), \qquad [5]$$

where $\mathrm{L}(\varepsilon - \varepsilon_n)$ is the lorentzian function

$$\mathrm{L}(\varepsilon - \varepsilon_n) = \frac{(\Gamma_n/2)^2}{(\varepsilon - \varepsilon_n)^2 + (\Gamma_n/2)^2} . \qquad [6]$$

Therefore, a resonance embedded in the continuum consists of a lorentzian lineshape with a full-width at half-maximum (FWHM) given by Γ_n.

Filtering. A suitable *test function* for the determination of the resonance properties of the system by means of the RTWPM[17,18] can be obtained by propagating an arbitrary wavepacket in time with the true hamiltonian, plus an asymptotic optical potential[19] which absorbs the non-resonant part of the spectrum.[15] The filtered wavepacket can now be represented as a linear superposition of the L^2 complex resonance eigenstates:

$$\Psi(q) \approx \sum_n b_n \varphi_n(q), \qquad [7]$$

where the b_n's are complex numbers. Since the model hamiltonian $\hat{\tilde{H}}$ is not hermitian, the states φ_n are not guaranteed to be orthogonal[20,21]. However, when the resonance peaks do not overlap significantly, they can be considered to be so with good approximation. Formally, the filtered wavepacket can also be expressed as a spectral expansion in terms of the continuum eigenstates of the true hamiltonian,

$$\Psi(q) = \int c(\varepsilon)\psi_\varepsilon(q)d\varepsilon\,. \qquad [8]$$

Spectrum. For the calculation of the resonance spectrum of the system employing the RTWPM,[15,17] the filtered test function (8) is propagated in time with the true hamiltonian $\hat{H}$ between t=-T and t=+T. Such propagated wavepacket is then used to construct a *time-autocorrelation function*, whose inverse Fourier transform yields the *spectral function*

$$\Omega_T(\varepsilon) \equiv \frac{1}{2\pi\hbar}\int_{-T}^{T}\langle\Psi(0)|\Psi(t)\rangle\exp(\imath\varepsilon t/\hbar)dt = |\,c(\varepsilon)\,|^2\,. \qquad [9]$$

On the other hand, when an analogous procedure is carried out propagating the test function (7) with the model hamiltonian $\hat{\tilde{H}}$, it is obtained that

$$\tilde{\Omega}_T(\varepsilon) \approx \sum_n |\,b_n\,|^2\,\mathrm{L}(\varepsilon-\varepsilon_n), \qquad [10]$$

provided the time T is long enough so that the lineshape function $\delta_T(\varepsilon)$ becomes much narrower than all the lorentzians $\mathrm{L}(\varepsilon-\varepsilon_n)$.[15,17,18] Eq. (10) shows that, for sufficiently long T, the calculated spectral function (9) consists of a series of approximately lorentzian resonances centered at the (real) peak eigenenergies, whose heights give the corresponding spectral weights as per $|\,b_n\,|^2 \approx \Omega_T(E_n)$.

Eigenfunctions. Once the peak resonance eigenenergies have been determined, the corresponding (real) continuum eigenfunctions can be calculated by[15,17]

$$\psi_{\varepsilon_n}(q) \approx \frac{1}{b_n}\frac{1}{2\pi\hbar}\int_{-T}^{T}\Psi(q,t)\exp(\imath\varepsilon_n t/\hbar)dt\,. \qquad [11]$$

RESULTS AND DISCUSSION

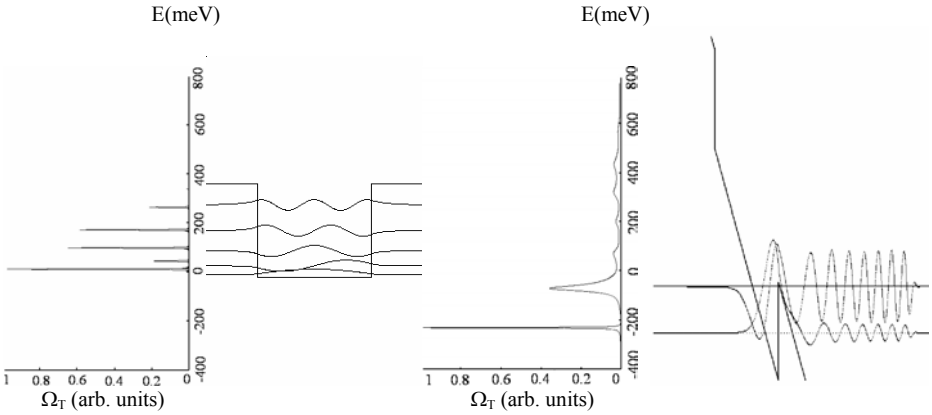
Calculations were performed for GaAs/$Ga_{1-x}Al_xAs$ rectangular QW's with a fixed Al concentration of x=0.45, yielding barriers of 336.69 meV and 224.56 meV for the conduction band (CB) and valence band (VB), respectively[18]. The effective masses of the electron and hole were taken as the GaAs effective masses, m_e*=0.0665m_e and m_h*=0.3024m_e, respectively[18]. The unfiltered test functions were chosen as narrow Gaussians placed inside the wells. The TDSE was integrated numerically, using the method explained in refs. [17,18]. The enforcement of the free boundary conditions necessary for systems with a continuum is always a vexing problem in numerical simulations. Here, the problem was solved by placing an absorbing (optical) potential[15,19,20] in the asymptotic region, $\mathrm{V_{opt}}(z) = i\gamma(z)$, with the smooth functional

form

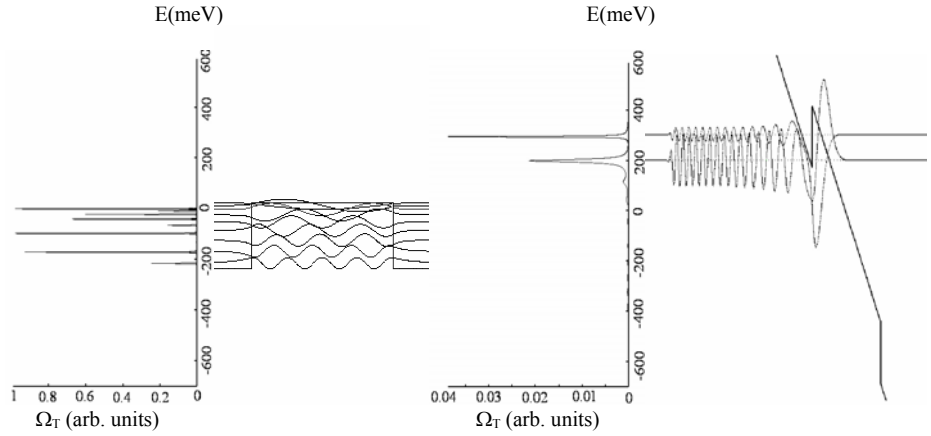
$$\gamma(z) = \frac{\gamma_{\max}}{2}\left[1 - \cos\frac{\pi(z - z_0)}{R}\right]. \qquad [12]$$

where $\gamma_{\max}$, z_0, and R are its maximum value, initial point, and range.

The figure below shows the CB spectral functions and corresponding peak resonance eigenfunctions for a 200 Å QW without an electric field (left), calculated with the methodology explained in ref. [18], and with an electric field of 400 kV/cm (right), calculated with this methodology. It is observed that the first bound state becomes a sharp, nearly lorentzian resonance, whereas the second state becomes a broad one, both of them strongly shifted in energy.

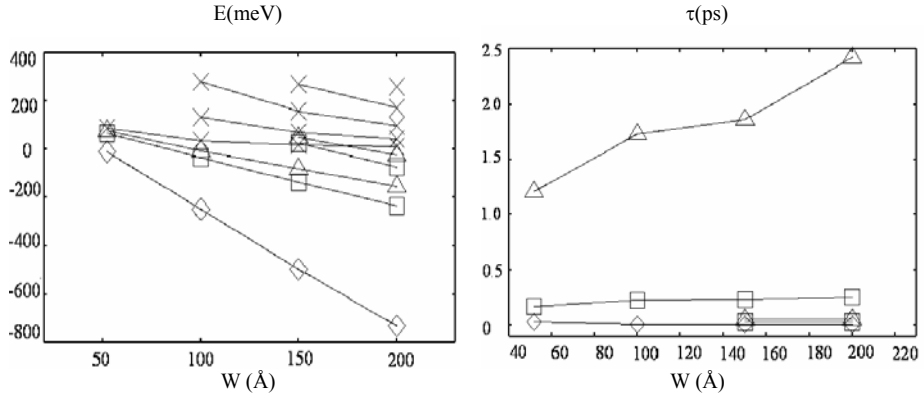


Inside the well, the eigenfunctions resemble the original bound ones, whereas outside they oscillate with an amplitude which is smaller the sharper the resonance. The second resonance is broad since it lies very close to the edge of the Stark well. Analogous remarks apply to the VB, which is displayed in the figure below.



The squeezing of the electron and hole eigenfunctions to the right and left of the well, respectively, indicates that the dc field causes a strong polarization of the exciton.

The lifetime of a resonance is defined and calculated in various ways.[10,14-16] Here, the FWHM was measured and employed in Eq. (3). The figure below shows the energies (left) and lifetimes (right) of the CB Stark resonances as functions of the width of the structure, W, and the strength of the field. The marks ×, △, ⟨, ◇, correspond to 0, 300, 400, 1000 kV/cm, respectively, and the lines connecting them are just a visual aid. The 200 Å QW, for example, presents five bound states without the field, two resonances for 300 and 400 kV/cm, and one resonance for 1000 kV/cm. It is seen that, whereas the bound eigenenergies decrease in an exponential fashion with W, the resonance peak energies decrease in an apparently linear manner. The lifetime, on the other hand, does not change much with W, especially at the higher fields.



CONCLUSIONS AND PERSPECTIVES

The present approach appears to be a valuable theoretical tool for accurate and systematic studies of low-dimensional semiconductor devices where tunneling plays an important role and where other common methodologies are not applicable. In the particular case of quantum wells, it was found that relatively strong dc fields (larger than 300 kV/cm) induce very large Stark shifts, electron-hole polarizations, and short carrier lifetimes. These results may be useful for the understanding and/or design of optoelectronic devices operating at high bias.

The RTWPM is being extended to the calculation of eigen and optical spectra without the constant effective-mass and single-hole-band approximations. Such studies will be reported elsewhere.

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