RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 34, NUMBER 12 15 DECEMBER 1986

Exact calculations of quasibound states of an isolated quantum well with uniform electric field: Quantum-well Stark resonance

D. Ahn and S. L. Chuang

Department of Electrical and Computer Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

(Received 1 October 1986)

We present universal plots from exact numerical calculations for the energy level and the resonance width of quasibound states in a quantum well with an applied electric field (quantum-well Stark resonance) by solving the Schrödinger equation directly. This calculation gives both the resonance positions and widths for the complex eigenvalue $E_0 - i\Gamma/2$ of the system. Our theory also shows that the energy shifts of the ground states for the electrons and holes have the same behaviors in high fields without any turnaround phenomenon, contrary to the results of Austin and Jaros.

Electronic and optical properties of quantum wells with applied external electric fields are of increasing interest. Studies of these areas are important both from a fundamental and a practical point of view. Optical modulators[1] and optical switching devices[2] based on the quantum confined Stark effect have been suggested. Possible device applications of the field-induced tunneling in quantum-well and quantum-barrier heterostructures include high-speed resonant tunneling devices.[3-6]

More recent theoretical studies[7-9] of the effects of external electric fields on the quantum-well systems have predicted both the field-induced level shifts and the field dependence of the carrier lifetime. In this paper, we report exact numerical calculations on quasibound states of a quantum well in an external electric field (quantum-well Stark resonance) by solving the Schrödinger equation for Stark resonance directly. It is found that the previous results based on phase-shift analysis[7,9] and the stabilization method[8] agree very well with our results over a wide range of the electric field. At an extremely high electric field, there is no turnaround behavior in the energy shift for both the electrons and the holes, contrary to the results in Ref. 7, where no explanation can be provided for that phenomenon. We believe that our direct numerical approach is very reliable even at a very high electric field, while the results using the phase-shift analysis may have drawbacks in the high-field limit. Our approach has an advantage over the previous results[7-9] in that both the Stark resonance position (quasibound-state level) and the width can be obtained from the single complex energy eigenvalue of the quantum-well Stark resonance problem. The disadvantage is that numerical subroutines of the Airy functions with complex arguments are required.

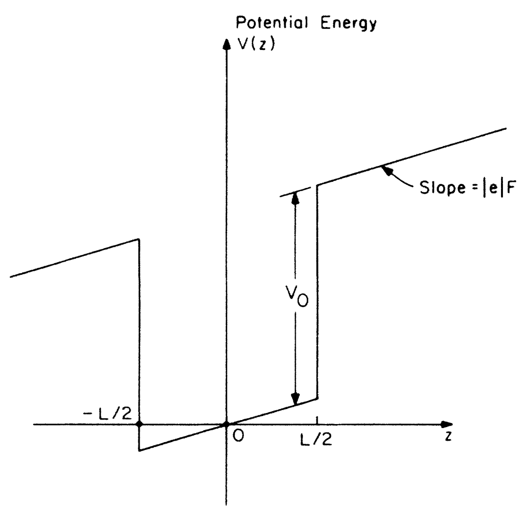

FIG. 1. Potential-energy profile $V(z)$ for a single quantum well with depth V_0 and width L subject to an external electric field F.

Consider an electron with charge $-|e|$ and effective mass m^*, in a finite quantum well of width L and depth V_0 in the presence of a constant electric field F along the positive direction of the well z (Fig. 1). We choose the origin to be at the center of the well. The Schrödinger equation of the system in the effective-mass approximation is given by[7,9]

$$
\begin{aligned}
&-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi(z)+|e|Fz\psi(z)=E\psi(z), \quad |z|\le L/2 , \\
&-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi(z)+(V_0+|e|Fz)\psi(z)=E\psi(z), \\
&\qquad\qquad |z|>L/2 .
\end{aligned} \tag{1}
$$

Since the potential energy term in Eq. (1) tends to $-\infty$ as z goes to $-\infty$, the system does not, strictly speaking, have true bound states.[7,10] In other words, the particle initially confined in a well can always lower its potential energy by tunneling out of the well when the field is not zero. It may happen, however, that the tunneling probability is very small. In such a case, we can regard the system as having quasibound states, in which the particles move "inside the well" for a considerable period of time and leave through tunneling only when a fairly long time interval τ has elapsed. In discussing the quasibound states, we may use the following formal method. Instead of considering the solutions of the Schrödinger equation with a boundary condition requiring the finiteness of the wave function at infinity, we shall look for solutions which represent outgoing waves at infinity;[10] this implies that the particle finally leaves the well by tunneling. Since such a boundary condition is complex, we cannot assert that the eigenvalues (energy) must be real. By solving the Schrödinger equation, we obtain a set of complex eigenvalues, which we write in the form

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

where Γ is found to be positive. E_0 and Γ correspond to the quasibound-state energy level and the resonance width, respectively. The tunneling probability per unit time is defined by

$$\omega = \Gamma/\hbar \;. \tag{3}$$

The solutions to Eq. (1) with the outgoing-wave condition are linear combinations of two independent Airy functions[11]

$$\psi(z) = \begin{cases} a_1[\mathrm{Bi}(\eta_2) + i\,\mathrm{Ai}(\eta_2)], & z < -L/2, \\ a_0\mathrm{Ai}(\eta_1) + b_0\mathrm{Bi}(\eta_1), & |z| \le L/2, \\ a_2\mathrm{Ai}(\eta_2), & z > -L/2 \;, \end{cases} \tag{4}$$

with

$$\eta_1 = -\left[\frac{2m^*}{(e\hbar F)^2}\right]^{1/3} (E - |e|Fz) \;, \tag{5a}$$

and

$$\eta_2 = -\left[\frac{2m^*}{(e\hbar F)^2}\right]^{1/3} (E - V_0 - |e|Fz) \;. \tag{5b}$$

The wave function for $z < -L/2$ represents an electron traveling to $z = -\infty$ after tunneling. The complex energy E can be found by solving the secular equation obtained by matching the value of ψ and its first derivative at the points, $z = \pm L/2$. The resulting determinantal equation is

$$\det \begin{bmatrix} \mathrm{Ai}(\eta_1^+) & \mathrm{Bi}(\eta_1^+) & -\mathrm{Ai}(\eta_2^+) & 0 \\ \mathrm{Ai}'(\eta_1^+) & \mathrm{Bi}'(\eta_1^+) & -\mathrm{Ai}'(\eta_2^+) & 0 \\ \mathrm{Ai}(\eta_1^-) & \mathrm{Bi}(\eta_1^-) & 0 & -[\mathrm{Bi}(\eta_2^-) + i\,\mathrm{Ai}(\eta_2^-)] \\ \mathrm{Ai}'(\eta_1^-) & \mathrm{Bi}'(\eta_1^-) & 0 & -[\mathrm{Bi}'(\eta_2^-) + i\,\mathrm{Ai}'(\eta_2^-)] \end{bmatrix} = 0 \;, \tag{6}$$

where $\eta_1^\pm$ and $\eta_2^\pm$ are the values of η_1 and η_2 evaluated at $z = L/2$ and $-L/2$, respectively. If we introduce a new parameter $E^{(0)}$ defined by

$$E^{(0)} = \frac{\hbar^2}{2m^*}\left[\frac{\pi}{L}\right]^2 \tag{7}$$

(which happens to be the ground-state energy of an infinite quantum well with width L), and define the normalized energy $\tilde{E} = E/E^{(0)}$, the normalized electric field $\tilde{F} = |e|FL/E^{(0)}$, and the normalized well depth $\tilde{V}_0 = V_0/E^{(0)}$, we may express $\eta_1^\pm$ and $\eta_2^\pm$ by these three normalized quantities: $\tilde{E}$, $\tilde{F}$, and $\tilde{V}_0$.

$$\eta_1^\pm = -\left[\frac{\pi^2}{\tilde{F}^2}\right]^{1/3} (\tilde{E} \mp \tfrac{1}{2}\tilde{F}) \;, \tag{8a}$$

$$\eta_2^\pm = -\left[\frac{\pi}{\tilde{F}^2}\right]^{1/3} (\tilde{E} - \tilde{V}_0 \mp \tfrac{1}{2}\tilde{F}) \;. \tag{8b}$$

This means that the solution of $\tilde{E}$ from Eq. (6) is universal and can be used for both electrons and holes with the replacement of the parameter $E^{(0)}$ with their corresponding effective masses.[12] (Here the effective masses inside and outside the well are assumed to be equal.) The normalized energy $\tilde{E}$ can be expressed in terms of only two normalized parameters, $\tilde{V}_0$ and $\tilde{F}$. Thus it is clear that both electrons and holes should have the same behaviors in their energy shift and the resonance width. To obtain the results of E_0

TABLE I. Comparison of the numerical results for $E_0 - i\Gamma/2$ using the exact numerical method of this paper, the phase-shift analysis (Refs. 7 and 9), and the stabilization method (Ref. 8).

F(kV/cm)		This paper (eV)	Phase-shift analysis (eV)	Stabilization method (eV)
75	E_0	0.025 167	0.025 167	0.025 167
	Γ	1.86×10^{-6}	1.9×10^{-6}	8.6×10^{-6}
100	E_0	0.024 2107	0.024 2105	0.024 2106
	Γ	3.64×10^{-5}	3.6×10^{-5}	4.1×10^{-5}
150	E_0	0.021 3716	0.021 3816	0.021 170
	Γ	6.41×10^{-4}	6.4×10^{-4}	6.5×10^{-4}

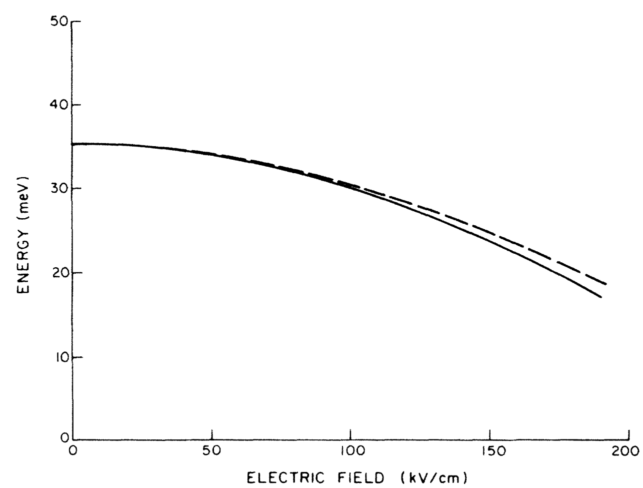

FIG. 2. Comparison of the ground-state energy of the variational calculation (Refs. 13 and 15) for infinite-well with appropriate effective-well width (dashed line) and the real part of the energy eigenvalue E_0 from exact calculation (solid line) of this paper.

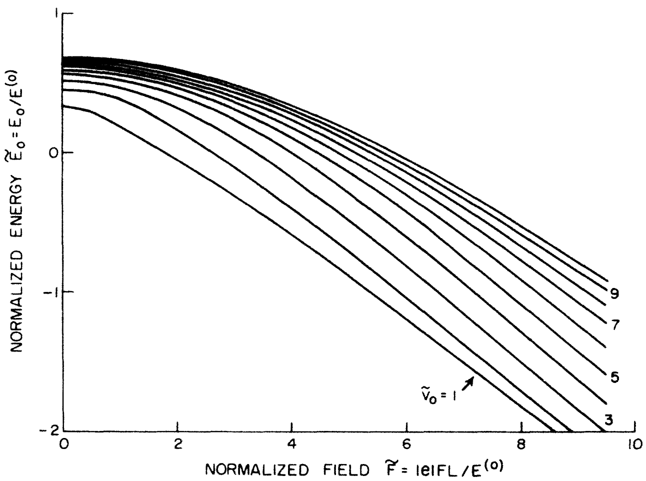

FIG. 3. The real part of the normalized energy $\tilde{E}_0 = E_0/E^{(0)}$ for various normalized well depths $V_0 = V_0/E^{(0)}$ is plotted vs the normalized electric field $\tilde{F} = |e|FL/E^{(0)}$.

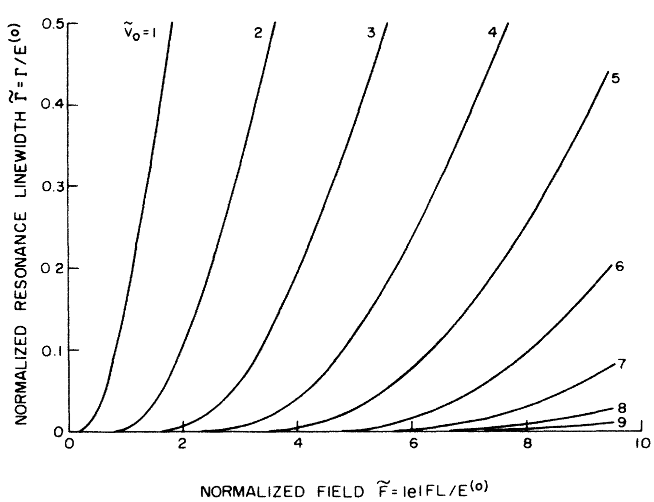

FIG. 4. The normalized resonance width $\tilde{\Gamma} = \Gamma/E^{(0)}$ for various $\tilde{V}_0$ is plotted vs normalized elecric field $\tilde{F} = |e|FL/E^{(0)}$.

and Γ for holes, one need only multiply $\tilde{E}$ by E_0 using the effective mass of the hole. We have solved Eq. (6) numerically to the desired accuracy using the series and asymptotic expansions of the Airy functions with complex arguments.[11] To check the validity of our approach, we compared our results with those of the previous methods[7,8] in Table I. The values of V_0, L, and m^* for the heavy holes used in the calculations are, respectively,

$$V_0 = 100\ \text{meV},\ L = 37\ \text{Å},\ m^* = 0.45 m_0\ , \qquad (9)$$

where m_0 is the free-electron mass. It is readily seen that our results agree very well with those of the phase-shift analysis[7,9] and the stabilization method.[8]

In Fig. 2, the real part of the energy E_0 (resonance position–solid line) for the ground-state energy with the values of V_0, L, and m^* for electrons given by $V_0 = 340$ meV, $L = 100$ Å, and $m^* = 0.0665 m_0$ is compared with the results of infinite-well variational calculations[13-15] (dashed lines), where we have used an effective well width $L_{\text{eff}} = 126.5$ Å, chosen to give the same E_0 at zero field for the variational calculations. It can be easily noticed that both calculations gave very similar results even up to 2×10^5 V/cm. However, the variational calculation for the infinite-well model cannot give the resonance width since no tunneling exists for the infinite well. The results of the normalized resonance energy $\tilde{E}_0 = E_0/E^{(0)}$ for various $\tilde{V}_0$ are plotted versus $\tilde{F}$ in Fig. 3. In contrast to the previous results[7] which are still controversial, the resonance position is found to be in the well even at very high field. The behaviors of the resonant position are the same for both electrons and holes with proper $E^{(0)}$ used together with Fig. 3 as discussed before. Thus the turnaround behavior for the holes and electrons in the energy shift shown in Ref. 7 is probably a drawback of that method itself. Using the same numerical values for holes as those in Ref. 7, $L = 30$ Å, $V_0 = 70$ meV, $m^* = 0.45 m_0$, we obtain $E^{(0)} = 92.26$ meV, $\tilde{V}_0 = 0.76$. We do not have any turnaround behavior even up to $\tilde{F} = 10$, or the electric field $F = 3075$ kV/cm, which covers a much wider range of electric field than that of Ref. 7. In Fig. 4, we plot the normalized resonance width $\tilde{\Gamma} = \Gamma/E^{(0)}$ for various $\tilde{V}_0$ vs $\tilde{F}$. Since the lifetime τ is defined by $\tau = \hbar/\Gamma$, the results plotted in Fig. 4 predict a rapid decrease of the carrier lifetime with increasing applied field by field enhanced tunneling.

In conclusion, we have solved the Schrödinger equation for a quantum well with uniform electric field directly. Complex eigenvalues for quantum-well Stark resonance are obtained. Our approach has an advantage over previous analyses[7-9] in that both the resonance position and width can be obtained from a single complex eigenvalue of the problem.

This work was partially supported by the Air Force, Contract No. F33615-84-K-1557 and the NASA Grant No. NAG 1-500. One of the authors (D.A.) would like to acknowledge the support of GTE.

[1]E. Tarucha and H. Okamoto, Appl. Phys. Lett. **48**, 1 (1986).
[2]D. A. B. Miller, D. S. Chemla, T. C. Damen, T. H. Wood, C. A. Burrus, A. C. Gossard, and W. Wiegmann, IEEE J. Quantum Electron. **21**, 1462 (1985).
[3]R. Tsu and L. Esaki, Appl. Phys. Lett. **22**, 562 (1973).
[4]A. R. Bonnefoi, D. H. Chow, and T. C. McGill, Appl. Phys. Lett. **47**, 886 (1985).
[5]F. Capasso, K. Mohammed, and A. Y. Cho, IEEE J. Quantum Electron. **22**, 1853 (1986).
[6]Y. Nakata, M. Asada, and Y. Suematsu, IEEE J. Quantum Electron. **22**, 1880 (1986).
[7]E. J. Austin and M. Jaros, Phys. Rev. B **31**, 5569 (1985).
[8]F. Borondo and J. Sánches-Dehesa, Phys. Rev. B **33**, 8758 (1986).

[9]E. J. Austin and M. Jaros, Appl. Phys. Lett. **47**, 274 (1985).

[10]L. D. Landau and E. M. Lifshitz, *Quantum Mechanics —Nonrelativistic Theory* (Pergamon, New York, 1981), pp. 555–560.

[11]*Handbook of Mathematical Functions*, edited by M. Abramowitz and I. A. Stegun (National Bureau of Standards, Washington, DC, 1964), pp. 446–452.

[12]M. Matsuura and T. Kamizato, Phys. Rev. B **33**, 8385 (1986).

[13]G. Bastard, E. E. Mendez, L. L. Chang, and L. Esaki, Phys. Rev. B **28**, 3241 (1983).

[14]D. A. B. Miller, D. S. Chemla, T. C. Damen, A. C. Gossard, W. Wiegmann, T. H. Wood, and C. A. Burrus, Phys. Rev. Lett. **53**, 2173 (1984).

[15]D. Ahn and S. L. Chuang, Appl. Phys. Lett. **49**, 1450 (1986).