Exact analytic analysis of finite parabolic quantum wells with and without a static electric field

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Exact analytic solutions of finite parabolic quantum wells are derived for both the unperturbed and the electric-field-applied cases. Several normalized parameters are defined so as to make our results universal within the scope of the envelope function approximation with a constant effective mass assumed. The Stark resonance position and the width in the electric-field-applied case can be obtained simultaneously from the complex eigenvalue $E_0 - i\Gamma/2$ of the system. By comparing the results calculated, respectively, by employing the exact solutions and the infinite-parabolic-well approximation, the validity of the approximation is rigorously examined. It is shown that the infinite-parabolic-well approximation is valid only under certain conditions as discussed in the text.

Recently, the parabolic quantum-well structures have received increased interest because of their various applications. Such structures have been successfully fabricated by using molecular-beam epitaxy with the band structure produced by employing both the superlattice grading technique[1–5] and the analog grading technique.[6] Although the former does in fact use superlattice structures to simulate parabolic quantum wells, its validity has been confirmed experimentally[1–5] and theoretically.[7] The photoluminescence and the electron-beam electroreflectance measurements of this system have been presented[1,2,6] to study the partitioning of the energy-gap discontinuities between the conduction and the valence bands. The structure has also been used in resonant tunneling to study its potential application in high-speed circuits.[5] Other applications include using it to design infrared detectors with low leakage currents and low electric-field sensitivity[8] and employing it as the graded barrier part of the quantum-well laser to improve the optical confinement factor and enhance the carrier collection into the thin quantum well so as to reduce the threshold current density.[9,10]

Due to its importance, many theoretical studies have been performed for it.[11–14] In these works, the eigenenergies are solved either numerically[11–13] or by assuming an infinite-parabolic-well depth.[14] When an electric field is present, a rigid boundary condition is always assumed[11–13] so that all states become bounded. Thus the linewidth broadening effect due to the electric field cannot be taken into account directly and the evaluation of a local one-dimensional density of states is required.[13,15] Furthermore, since the wave functions are forced to be zero at the rigid boundaries, some inaccuracy must be produced.

In this paper, we will give the exact analytic solutions of a finite parabolic quantum well with a uniform electric field present or not. The solutions are within the scope of the envelope function approximation[16] and a constant effective mass is assumed. When an electric field is applied, we can simultaneously obtain the Stark resonance position and the width from the single complex eigenenergy. We also define several normalized parameters and express the analytic wave functions by these parameters so that our results are universal. By comparing our results with those obtained by the infinite-parabolic-well approximation, we have a clear picture about the validity of the latter.

Consider an electron with charge $-|e|$ and effective mass m^* in a finite parabolic quantum well of half-width a and depth V_0 in the presence of a uniform electric field F along z, as shown in Fig. 1. The time-independent Schrödinger equation for such a system is given by

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi(z)+\left[V_0\left[\frac{z}{a}\right]^2+|e|Fz\right]\psi(z)=E\psi(z)\ ,\qquad |z|\le a\ ,\tag{1}$$

$$-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}\psi(z)+(V_0+|e|Fz)\psi(z)=E\psi(z)\ ,\quad |z|>a\ .\tag{2}$$

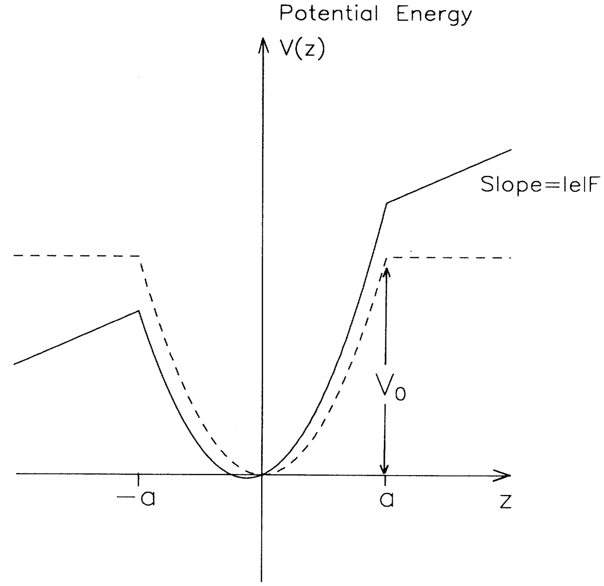

FIG. 1. Potential-energy profiles of the finite parabolic quantum-well structures investigated in this paper. The depth and the width are V_0 and $2a$, respectively.

The eigenvalue E here should be a complex number expressed as

$$E=E_0-i\Gamma/2\ , \tag{3}$$

where E_0 and Γ correspond to the energy level and the resonance width of the quasibounded states, respectively. If there is no applied field, then $E=E_0$ which is a real number. Defining $Z=z/a$ and substituting this relation into the above equations, we get

$$\frac{d^2}{dZ^2}\psi(Z)+(\tilde{U}^2-\tilde{F}Z-\tilde{V}^2Z^2)\psi(Z)=0\ ,\quad |Z|\le 1\ , \tag{4}$$

$$\frac{d^2}{dZ^2}\psi(Z)+(\tilde{U}^2-\tilde{F}Z-\tilde{V}^2)\psi(Z)=0\ ,\quad |Z|>1\ , \tag{5}$$

where

$$\tilde{U}^2=\frac{2m^*a^2E}{\hbar^2}\ , \tag{6}$$

$$\tilde{V}^2=\frac{2m^*a^2V_0}{\hbar^2}\ , \tag{7}$$

$$\tilde{F}=\frac{2m^*|e|Fa^3}{\hbar^2}\ . \tag{8}$$

The parameters $\tilde{U}$, $\tilde{V}$, and $\tilde{F}$ are the normalized well parameter, the normalized structure parameter, and the normalized field parameter, respectively. They are defined similar to the normalized parameters of optical waveguides.[18,19]

First, we consider the $\tilde{F}=0$ case, i.e., no applied electric field. The normalized equations become

$$\frac{d^2}{dZ^2}\psi(Z)+(\tilde{U}^2-\tilde{V}^2Z^2)\psi(Z)=0\ ,\quad |Z|\le 1\ , \tag{9}$$

$$\frac{d^2}{dZ^2}\psi(Z)-\tilde{W}^2\psi(Z)=0\ ,\quad |Z|>1\ , \tag{10}$$

where $\tilde{W}$ is defined as $[2m^*a^2(V_0-E)/\hbar^2]^{1/2}$ (barrier parameter). Solutions of the second equation are clearly the exponential functions, so we focus on the first equation. The form of this equation is the same as that of the TE modes in a cladded-parabolic planar optical waveguide. Solutions of the optical waveguide have been given in Ref. 19. However, the final form in the reference is wrong, so we would like to derive the exact solutions for the quantum-well case again and give the correct final form. Assuming that $\psi(\zeta)=\exp(-\zeta/2)\phi(\zeta)$, where $\zeta=\tilde{V}Z^2$, and substituting this form into the corresponding equation, we obtain

$$\zeta\frac{d^2\phi}{d\zeta^2}+(\tfrac{1}{2}-\zeta)\frac{d\phi}{d\zeta}-\frac{1}{4}\left[1-\frac{\tilde{U}^2}{\tilde{V}}\right]\phi=0\ . \tag{11}$$

The solutions to this equation are the confluent hypergeometric functions[20] $M(\alpha,\beta,\zeta)$ and $U(\alpha,\beta,\zeta)$, with $\alpha=(1-\tilde{U}^2/\tilde{V})/4$ and $\beta=\frac{1}{2}$. The solution that involves only $M(\alpha,\beta,\zeta)$ is that for the even states, and the one that involves only $U(\alpha,\beta,\zeta)$ is for the odd states. Now we can write the solution in each region in the proper form:

$$\psi(Z)=\begin{cases} C_1\exp(-\tilde{V}Z^2/2)\phi(\tilde{V}Z^2)\ , & |Z|\le 1\ ,\\ C_2\exp[-\tilde{W}(|Z|-1)]\ , & |Z|>1\ ,\end{cases} \tag{12}$$

where $\phi(\tilde{V}Z^2)$ is $M(\alpha,\beta,\tilde{V}Z^2)$ or $U(\alpha,\beta,\tilde{V}Z^2)$ depending on the parity of the state. By requiring that the wave functions itself and its first derivative be continuous at the boundaries, we have the following transcendental equation:

$$2\phi'(\tilde{V})-\left[1-\frac{\tilde{W}}{\tilde{V}}\right]\phi(\tilde{V})=0\ . \tag{13}$$

Solving this equation gives the eigenenergies.

If $\tilde{F}\neq 0$, the independent solutions of the well part are given by[11,20]

$$\psi_1(\xi)=\exp\left[-\frac{\xi^2}{4}\right]M(\tfrac{1}{2}\gamma+\tfrac{1}{4},\tfrac{1}{2},\tfrac{1}{2}\xi^2)\ , \tag{14}$$

$$\psi_2(\xi)=\xi\exp\left[-\frac{\xi^2}{4}\right]M(\tfrac{1}{2}\gamma+\tfrac{3}{4},\tfrac{3}{2},\tfrac{1}{2}\xi^2)\ , \tag{15}$$

where

$$\xi=\sqrt{2}\tilde{V}^{-1/2}\left[\tilde{V}Z+\frac{1}{2}\frac{\tilde{F}}{\tilde{V}}\right]\ , \tag{16}$$

$$\gamma=-\frac{1}{2\tilde{V}}\left[\tilde{U}^2+\frac{1}{4}\frac{\tilde{F}^2}{\tilde{V}^2}\right]=-\frac{1}{2\tilde{V}}\left[\tilde{V}^2\tilde{E}+\frac{1}{4}\frac{\tilde{F}^2}{\tilde{V}^2}\right]\ . \tag{17}$$

The normalized energy $\tilde{E}$ is defined as $\tilde{E}=\tilde{U}^2/\tilde{V}^2$. Note that the complex eigenenergy is included in the parameter γ, thus a subroutine capable of calculating complex confluent hypergeometric functions is required. For the wave functions in the barrier region, we adopt the solutions proposed in Ref. 17 to account for the tunneling effect. The wave function of the system is then given by

$$\psi(Z)=\begin{cases} a_1[\mathrm{Bi}(\eta)+i\,\mathrm{Ai}(\eta)]\ , & Z<-1\ ,\\ a_0\psi_1(\xi)+b_0\psi_2(\xi)\ , & |Z|\le 1\ ,\\ a_2\mathrm{Ai}(\eta)\ , & Z>1\ ,\end{cases} \tag{18}$$

where $\eta=\tilde{F}^{1/3}(Z+\tilde{W}^2/\tilde{F})$ and Ai,Bi are the independent Airy functions.[20] To get the eigenenergies, we require that both the wave function and its first derivative be continuous at the boundaries between the well and the barrier regions and solve the resultant secular equation. The equation is given by

$$\det\begin{bmatrix} \psi_1(\xi^+) & \psi_2(\xi^+) & -\mathrm{Ai}(\eta^+) & 0\\ \psi_1'(\xi^+) & \psi_2'(\xi^+) & -\mathrm{Ai}'(\eta^+) & 0\\ \psi_1(\xi^-) & \psi_2(\xi^-) & 0 & -[\mathrm{Bi}(\eta^-)+i\,\mathrm{Ai}(\eta^-)]\\ \psi_1'(\xi^-) & \psi_2'(\xi^-) & 0 & -[\mathrm{Bi}'(\eta^-)+i\,\mathrm{Ai}'(\eta^-)]\end{bmatrix}=0\ , \tag{19}$$

where $\xi^{\pm}$ and $\eta^{\pm}$ are the values of ξ and η evaluated at $z=a(Z=1)$ and $z=-a(Z=-1)$, respectively. Note that the derivatives of the functions are calculated with respect to z, thus some proper factors must be included to give the correct results. Also note that with the normalized parameters defined before $(\tilde{U},\tilde{V},\tilde{W},\tilde{E},\tilde{F})$, all of the solutions have been expressed by them, thus the results obtained are universal for both electrons and holes in all cases.

After obtaining the exact solutions, we can now see some numerical examples. First, we investigate the validity of the infinite-parabolic-well approximation with no applied electric field by comparing the exact results with those predicted by the approximation. The results are shown in Fig. 2. The x and y axes are the structure parameter $\tilde{V}$ and the normalized energy $\tilde{E}$, respectively. We find that the effect of the finite-parabolic-well depth is to lower the energies of the states. At the "cutoff" region of each state, the energy difference between the exact and the approximate results of the state is quite large. However, for the states whose energies are lower than the mentioned state, the energy differences are not so obvious. The largest error occurs at the cutoff region of the ground state. As the value of $\tilde{V}$ increases, this error becomes smaller. The reason for this phenomenon is that as $\tilde{V}$ becomes larger the effect of the barrier becomes more insignificant, thus the eigenenergies of the lower states given by the approximation are closer to the exact values. Consequently, if the infinite-parabolic-well approximation is adopted for its simplicity, the energies of the several lowest states calculated by using the approximation will be acceptable only when $\tilde{V}$ is sufficiently large.

When an electric field is applied, a parabolic quantum well becomes leaky so that there are no true bound states.[17] For such a system, it is instructive to compare it with the rectangular case[17] with the same parameters to see the effects of the different well shapes. The parameters are $a=18.5$ Å, $m^*=0.45m_0$, and $V_0=100$ meV. The complex eigenenergies of the ground state of both systems are shown in Table I. It is clear that the energy level of the finite parabolic well is substantially higher than that of the rectangular well. Due to this higher-energy level, the resonance width of the parabolic well is much larger than that of the rectangular case. It should be noticed that the energy-level shifts of the both cases are about the same in contrast to their large energy-level difference. We also see that the infinite-parabolic-well approximation produces substantial errors for this case. Furthermore, it cannot give the resonance width. Therefore, for the electric-field applied case, the infinite-parabolic-well approximation may have only limited use.

To see the electric-field dependence of the ground state of a finite parabolic well, we calculate the variation of the normalized energy level $\tilde{E}_0=E_0/V_0$ and the normalized resonance width $\tilde{\Gamma}=\Gamma/V_0$ with respect to the normalized field magnitude $\tilde{F}$ and show the results in Figs. 3 and 4, respectively. The energy level decreases with the increase of the electric field as expected. For the well of larger $\tilde{V}$, the unperturbed value of $\tilde{E}_0$ is smaller than that of a well with smaller $\tilde{V}$ and the slope of the $\tilde{E}_0$ curve is smaller. The normalized resonance width $\tilde{\Gamma}$ increases rapidly with the electric field which means that the lifetime τ defined as $\tau=\hbar/\Gamma$ has a rapid decrease with the electric field. As $\tilde{V}$ increases, the increasing rate of $\tilde{\Gamma}$ with respect to $\tilde{F}$ becomes smaller.

As the last example, we would like to investigate a case where two states exist. The structure parameter $\tilde{V}$ of this case is 4. The variations of $\tilde{E}_0$ and $\tilde{\Gamma}$ with respect to $\tilde{F}$ are shown in Fig. 5. It is shown that the $\tilde{E}_0$ curves are rather smooth compared with the corresponding curves in the previous example. We also find that the $\tilde{\Gamma}$ values

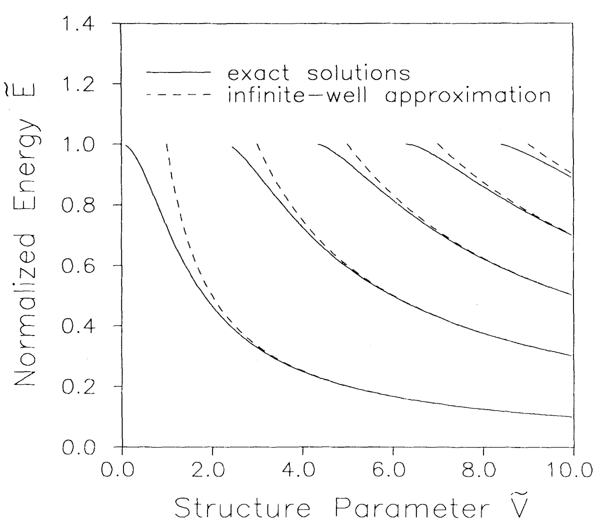

FIG. 2. Normalized energies $\tilde{E}=E/V_0$ of an unperturbed finite parabolic quantum well are plotted vs the structure parameter $\tilde{V}$. Solid: exact solutions. Dashed: infinite-parabolic-well approximation.

TABLE I. Comparison of the numerical results for $E_0-i\Gamma/2$ of a rectangular and a parabolic quantum well. The results for the parabolic quantum well are calculated by using the exact solutions and the infinite-parabolic-well approximation, respectively. The results for the rectangular well are the same as those presented in Ref. 17.

F (kV/cm)		Rectangular (meV)	Finite parabolic (meV)	Infinite parabolic (meV)
0	E_0	26.339 668	46.349 216	49.737 462
	Γ	0	0	0
	ΔE_0	0	0	0
75	E_0	25.166 733	45.204 518	49.256 173
	Γ	0.001 862	0.072 398	0
	ΔE_0	−1.172 935	−1.144 698	−0.481 289
100	E_0	24.210 554	44.236 741	48.881 831
	Γ	0.036 386	0.435 238	0
	ΔE_0	−2.129 114	−2.112 475	−0.855 625
150	E_0	21.371 354	41.792 427	47.812 306
	Γ	0.641 014	2.467 412	0
	ΔE_0	−4.968 314	−4.556 789	−1.925 156

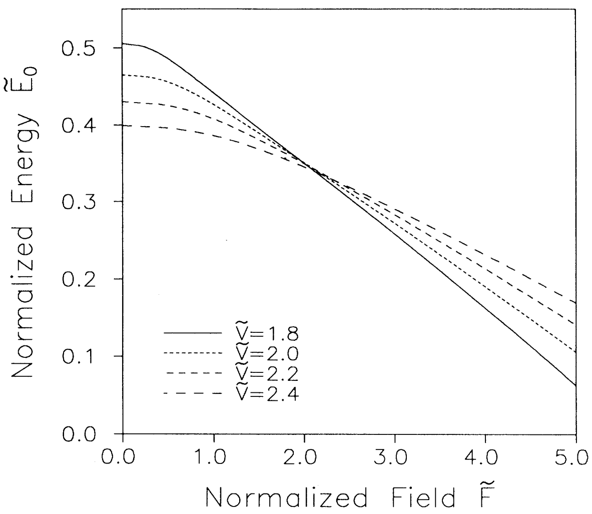

FIG. 3. The normalized energy level $\tilde{E}_0 = E_0/V_0$ for various structure parameters $\tilde{V}$ is plotted vs the normalized electric field $\tilde{F}$.

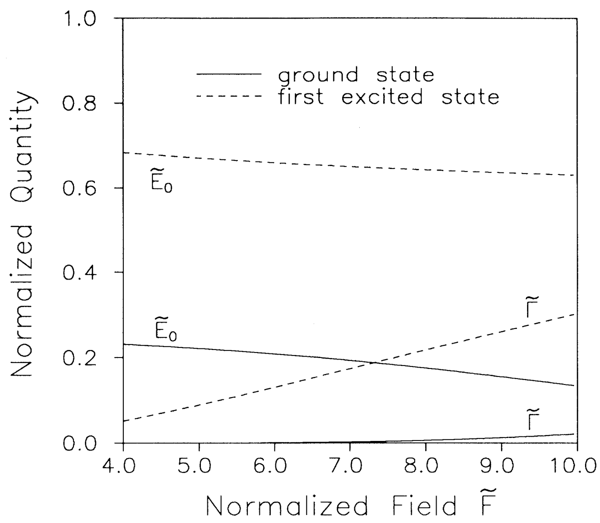

FIG. 5. The normalized energy level $\tilde{E}_0$ and the normalized resonance width $\tilde{\Gamma}$ of a two-state parabolic quantum well ($\tilde{V}=4$) are plotted vs the normalized electric field $\tilde{F}$.

of the ground state are much smaller than those of the first excited state. This is due to the fact that the effective barrier width for the ground state is much thicker than that for the first excited state. For such a multistate quantum well, the infinite-parabolic-well approximation predicts that the energy-level shifts are equal for all of the states of a well.[14] To investigate the correctness of this point, we calculate the normalized energy-level shifts $\Delta\tilde{E}_0$ of the two states as functions of the normalized field strength $\tilde{F}$ by using the exact solutions and the infinite-parabolic-well approximation and show the results in Fig. 6. It clearly shows that the differences between the exact and the approximate values are quite large especially for the excited state or when the field is strong. Only when the electric field is weak and for the ground state are the approximate values acceptable. Based on the comparison made here and that given in the first example, we may conclude that the infinite-parabolic-well approximation is valid only for the several lowest states of a given parabolic quantum well. The number of the several lowest states depends on the value of $\tilde{V}$ and the strength of the applied field $\tilde{F}$. In general, the larger the $\tilde{V}$ is and the smaller the $\tilde{F}$ is, the more states the infinite-parabolic-well approximation can accurately predict. However, the infinite-parabolic-well approximation can never give the resonance width.

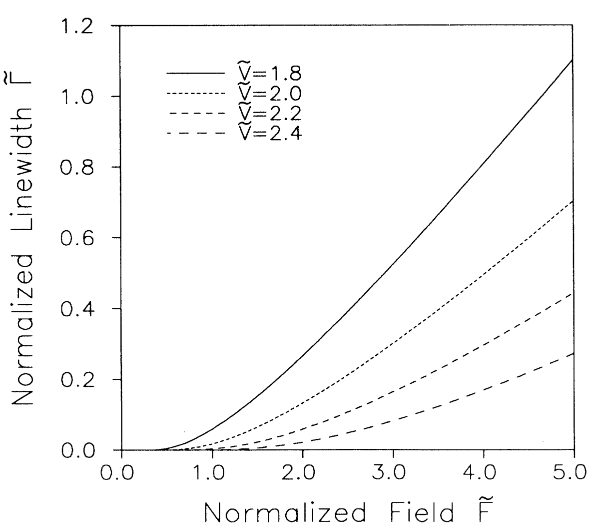

FIG. 4. The normalized resonance width $\tilde{\Gamma} = \Gamma/V_0$ for various structure parameters $\tilde{V}$ is plotted vs the normalized electric field $\tilde{F}$.

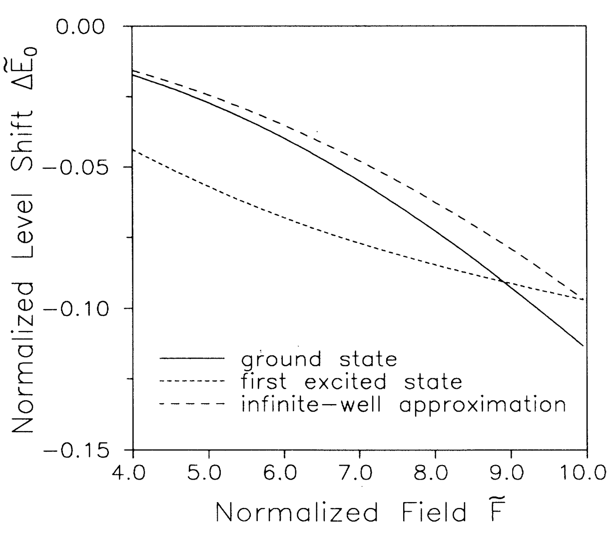

FIG. 6. The normalized energy-level shifts $\Delta\tilde{E}_0 = \Delta E_0/V_0$ of the two-state parabolic quantum well are plotted vs the normalized electric field $\tilde{F}$. Solid: exact solutions. Dashed: infinite-parabolic-well approximation.

In this paper, we have derived exact analytic solutions for the finite parabolic quantum well with and without the electric field present. By comparing the exact results with those calculated by the infinite-parabolic-well approximation, the validity of the approximation has been rigorously examined. Since the finite parabolic quantum-well structure has wide applications, the study given here should be valuable for the understanding of the designing for the cases where the structure is involved.

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