Enhancement of nonparabolicity effects in a quantum well

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The effects of conduction-band nonparabolicity on the confinement energy and energy dispersion parallel to the layers for a GaAs quantum well are investigated with the use of an expression for the bulk conduction-band dispersion expanded to fourth order in k. The anisotropy of the conduction band is included. We derive some accurate analytical expressions for the perpendicular mass, which gives the confinement energy, and the parallel mass, which is relevant for motion along the quantum well. These masses explicitly depend on the confinement energy. We find that the nonparabolicity enhancement for the parallel mass is about three times stronger than for the perpendicular mass. We finally compare with some recent experimental results.

I. INTRODUCTION

The energy of the bottom of an electron subband in a quantum well can often be determined to a reasonable accuracy by a simple particle-in-a-box calculation with the kinetic energy given by $\hbar^2k^2/2m$. For subbands fairly far from the bulk conduction-band edge, corrections due to the nonparabolicity of the conduction band can be important. Several schemes[1-4] have been proposed to take these nonparabolicity effects into account. Rössler[5] has shown that it is necessary to include the second $(\Gamma_8+\Gamma_7)$ conduction band in addition to the lowest conduction band, the heavy- and light-hole bands, and the split-off band for an accurate description of the dispersion of the conduction band more than 50 meV above the band edge.

While the nonparabolicity effects on the confinement energies have been considered by several authors, the dispersion parallel to the layers $E(\mathbf{k}_\parallel)$ of the electron subbands has received less attention. For hole subbands it has been shown[6] that the combination of confinement and coupling between the heavy-hole and light-hole bands causes a highly nonparabolic $E(\mathbf{k}_\parallel)$ dispersion, which is very different from that in the bulk. The $E(\mathbf{k}_\parallel)$ dispersion of the electron subbands is roughly parabolic, but it is conceivable that the degree of nonparabolicity can be different in quantum wells compared to the bulk.

In this Brief Report we derive expressions for the confinement energies and the $E(\mathbf{k}_\parallel)$ dispersion in a GaAs quantum well starting from an accurate expression of the bulk conduction band. We include the anisotropy of the conduction band but neglect the spin splitting. The main result is that the nonparabolicity correction to the curvature at the bottom of a subband with a certain confinement energy is more than 3 times stronger than the corresponding correction to the confinement energy.

II. THEORY

Using a 14-band $\mathbf{k}\cdot\mathbf{p}$ theory Braun and Rössler[7] have shown that the bulk conduction-band dispersion expanded to fourth order in k is given by the expression

$$E(\mathbf{k})=\hbar^2k^2/2m_1+\alpha_0k^4+\beta_0(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)\pm\gamma_0[k^2(k_x^2k_y^2+k_y^2k_z^2+k_z^2k_x^2)-9k_x^2k_y^2k_z^2)]^{1/2}\ , \tag{1}$$

where $m_1=0.0665$ (in units of the free-electron mass, which we henceforth set equal to 1) is the effective electron mass, $\alpha_0=-1.969\times10^{-29}$ eV cm^4, $\beta_0=-2.306\times10^{-29}$ eV cm^4, and $\gamma_0=-2.8\times10^{-23}$ eV cm^3 for GaAs. The term proportional to β_0 describes the anisotropy of the conduction band while the last term gives the spin splitting which is due to the violation of inversion symmetry in GaAs.

If we neglect the spin splitting and collect the k_z terms separately, we can write

$$E(\mathbf{k})=\alpha_0k_z^4+\left[\frac{\hbar^2}{2m_1}+(2\alpha_0+\beta_0)(k_x^2+k_y^2)\right]k_z^2+\frac{\hbar^2}{2m_1}(k_x^2+k_y^2)+(2\alpha_0+\beta_0)k_x^2k_y^2+\alpha_0(k_x^4+k_y^4)\ . \tag{2}$$

We assume that the layered structure is grown along the [001] direction, replace k_z by $-id/dz$, and add the potential $V(z)$ of the quantum well. Since we have translational invariance parallel to the quantum well, k_x and k_y remain good quantum numbers. We first determine the confinement energies $[k_\parallel\equiv(k_x^2+k_y^2)^{1/2}=0]$.

It is easily verified that the solutions of the Schrödinger equation in the nonparabolic case are still of the form $\cos(Kz)$ or $\sin(Kz)$ (in the well) and $\exp(-\lambda\,|\,z\,|\,)$ (in the barriers) but now we have the following relation between the confinement energy $\varepsilon\equiv E(k_\parallel=0)$ and the parameter K:

$$\varepsilon=\alpha_0K^4+\hbar^2K^2/2m_1\ . \tag{3}$$

For the $Al_xGa_{1-x}As$ barriers it would be appropriate to extract the decay constant λ as a function of energy below the bulk conduction-band edge from a calculation of the complex band structure of $Al_xGa_{1-x}As$. (See, e.g., Refs. 2 and 4.) Since the energy levels for a quantum well are fairly insensitive to the properties of the barrier material[2] (unless the quantum well is very narrow) we have neglected the nonparabolicity effects in $Al_xGa_{1-x}As$. Here we thus set α_0 and β_0 equal to zero and find

$$\lambda=[2m_2(V_0-\varepsilon)]^{1/2}/\hbar \ . \tag{4}$$

V_0 is the conduction-band discontinuity between GaAs and $Al_xGa_{1-x}As$ and m_2 is the effective mass in $Al_xGa_{1-x}As$. We use boundary conditions with continuity of the envelope wave function and its derivative divided by the effective mass in the bulk.[8] This leads to the transcendental equations

$$\tan(Kb)=\frac{m_1\lambda}{m_2K} \quad \text{(even parity)} \tag{5a}$$

and

$$\cot(Kb)=-\frac{m_1\lambda}{m_2K} \quad \text{(odd parity)} \ , \tag{5b}$$

where b is half the well width. To solve Eqs. (5a) and (5b) we must invert Eq. (3) and express K in terms of ε. It is sometimes convenient to express the results in terms of two constants, α' and β' defined by

$$\alpha' \equiv -(2m_1/\hbar^2)^2\alpha_0 \tag{6a}$$

and

$$\beta' \equiv -(2m_1/\hbar^2)^2\beta_0 \ . \tag{6b}$$

They have the values $\alpha'=0.600$ eV^{-1} and $\beta'=0.702$ eV^{-1}. We find

$$K=\left[\frac{m_1}{\alpha'\hbar^2}[1-(1-4\alpha'\varepsilon)^{1/2}]\right]^{1/2} . \tag{7}$$

For most energies of interest $\alpha'\varepsilon \ll 1$ and we obtain

$$K \approx [2m_1\varepsilon(1+\alpha'\varepsilon)]^{1/2}/\hbar \ . \tag{8}$$

From this relation it is reasonable to define an energy-dependent perpendicular mass[9]

$$m_\perp^* \approx m_1(1+\alpha'\varepsilon) \tag{9}$$

or, more accurately,

$$m_\perp^*=\frac{m_1}{2\alpha'\varepsilon}[1-(1-4\alpha'\varepsilon)^{1/2}] \ , \tag{10}$$

using Eq. (7). It is easy to verify that it is the same as the similarly defined energy-dependent bulk mass in the [001] direction. A commonly used expression for an energy-dependent effective mass was derived by Kolbas:[10]

$$m(E)=0.0665+0.0436E+0.236E^2-0.147E^3 \ , \tag{11}$$

where E is in eV. To lowest order this corresponds to $\alpha'=0.656$ eV^{-1}. This mass is thus close to the perpendicular mass $m_\perp^*$ given by Eq. (9).

The expressions above can be generalized to the case when k_x and k_y are different from zero. If we replace k_z by K in Eq. (2) and invert this expression we can express K in terms of E, k_x, and k_y:

$$K=\left\{G_1\left[1-\left[1-\frac{G_2}{G_1^2}\right]^{1/2}\right]\right\}^{1/2} , \tag{12}$$

where

$$G_1=\frac{m_1}{\alpha'\hbar^2}-\frac{2\alpha'+\beta'}{2\alpha'}k_\parallel^2 \tag{13a}$$

and

$$G_2=\frac{4m_1^2E}{\alpha'\hbar^4}-\frac{2m_1}{\alpha'\hbar^2}k_\parallel^2+k_\parallel^4+\frac{\beta'}{\alpha'}k_x^2k_y^2 \ . \tag{13b}$$

λ is now given by

$$\lambda=[2m_2(V_0-E)/\hbar^2+k_\parallel^2]^{1/2} \ . \tag{14}$$

The transcendental equations [(5a) and (5b)] can be solved numerically for different values of k_x and k_y and in this way we can determine the energy dispersion $E(\mathbf{k}_\parallel)$.

Although this procedure is straightforward, it is not very illuminating, and a reasonable approximation, which gives the curvature at the bottom of a subband in analytical form, is desirable. One such approximation is to determine the confinement energies (for $k_\parallel=0$) numerically from Eqs. (5a) and (5b) with the use of (4) and (7) and then treat the other terms in Eq. (2)

$$(2\alpha_0+\beta_0)k_\parallel^2k_z^2+\hbar^2k_\parallel^2/2m+\alpha_0k_\parallel^4+\beta_0k_x^2k_y^2 \tag{15}$$

in first-order perturbation theory. It is convenient to express the results in terms of the probability P_w (P_b) that the electron is in the well (barrier) given by

$$P_w=\frac{b+t\sin(2Kb)/2K}{b+t\sin(2Kb)/2K+[1+t\cos(2Kb)]/2\lambda} \ , \tag{16a}$$

$$P_b=\frac{[1+t\cos(2Kb)]/2\lambda}{b+t\sin(2Kb)/2K+[1+t\cos(2Kb)]/2\lambda} \ , \tag{16b}$$

where $t=+1$ (-1) for states with even (odd) parity. The expectation value of expression (15) becomes

$$\left[(2\alpha_0+\beta_0)K^2P_w+\frac{\hbar^2}{2m_1}P_w+\frac{\hbar^2}{2m_2}P_b\right]k_\parallel^2 + \alpha_0P_wk_\parallel^4+\beta_0P_wk_x^2k_y^2 \ . \tag{17}$$

The terms $(\hbar^2/2m_1)P_w+(\hbar^2/2m_2)P_b$ describe the mass enhancement which is due to the penetration of the wave function into the barrier and occurs even in the absence of nonparabolicity.[11] The coefficient in front of $k_\parallel^2$ becomes

$$\frac{\hbar^2}{2m_1}\left[P_w+\frac{m_1}{m_2}P_b-(2\alpha'+\beta')\frac{\hbar^2K^2}{2m_1}P_w\right] . \tag{18}$$

It is reasonable to define an energy-dependent parallel mass $m_\parallel^*(E)$ by identifying (18) with $\hbar^2/2m_\parallel^*(E)$. It can be shown[12] that $m_\parallel^*$ is equal to the cyclotron mass in the limit when the magnetic field goes to zero. The cyclotron mass is also found to increase with magnetic field. However, to include this effect properly one needs an expression for the bulk dispersion up to sixth order in k. It would contain terms proportional to $k_z^2k_\parallel^4$, which could give a sizable correction to the B^2 term for the Landau levels.

We can find simpler approximations from Eq. (18), which we first rewrite

$$\frac{\hbar^2}{2m_1}\left[1-(2\alpha'+\beta')\frac{\hbar^2K^2}{2m_1} - P_b\left[\frac{m_2-m_1}{m_2}-(2\alpha'+\beta')\frac{\hbar^2K^2}{2m_1}\right]\right] . \quad (19)$$

The first two terms correspond to the approximation of replacing k_z in Eq. (2) by K given by Eq. (7). It is seen that the correction is the probability that the particle is in the barriers (which usually is a few percent) multiplied by the difference between two terms of similar order of magnitude. Neglecting this correction and expanding K^2 to the lowest order in ε, we obtain

$$(\hbar^2/2m_1)[1-(2\alpha'+\beta')\varepsilon] . \quad (20)$$

By equating this to $\hbar^2/2m_\parallel^*$ we thus obtain a remarkably simple expression for $1/m_\parallel^*$ where the nonparabolicity correction is proportional to the confinement energy. Comparison with Eq. (9) shows that in this approximation the ratio of the nonparabolicity corrections for $1/m_\parallel^*$ and for $1/m_\perp^*$ becomes about $(2\alpha'+\beta')/\alpha' \approx 3.2$.

III. RESULTS AND CONCLUSIONS

We consider GaAs quantum wells between $Al_{0.4}Ga_{0.6}As$ barriers, take the conduction-band discontinuity to be 324 meV [65% of the energy-gap difference between $Al_{0.4}Ga_{0.6}As$ and GaAs (Ref. 13)], and use $m_2=0.0999$ for the mass in the barrier.[13]

In Fig. 1 we show the $E(\mathbf{k}_\parallel)$ dispersion for the lowest subband in a 50-Å quantum well in the [100] direction for three different cases: (*a*) a numerical solution of Eqs. (5a) and (5b) together with Eqs. (12)–(14), (*b*) nonparabolic bands with the approximate first-order perturbation expression (20), and (*c*) parabolic bands. We see that the perturbation expression (*b*) is a quite good approximation to the exact curve (*a*). It is found that expression (18) gives a curve which on the scale of Fig. 1 is indistinguishable from the exact result (*a*).

In Fig. 2 we show the parallel mass $m_\parallel^*$ and the perpendicular mass $m_\perp^*$ for the lowest subband as a function of well width in comparable approximations. Both the masses increase when the well width is decreased, but the ratio between their enhancements remains almost constant, somewhat larger than 3.

Recent interband magneto-optical experiments with an 80-Å quantum well,[14] for which this calculation gives $m_\parallel^*=0.073$, could indeed be quantitatively explained only if an 11% higher electron mass were used as input for a six-band model. Since this model (including conduction, heavy-hole and light-hole bands, and spin) to some extent includes nonparabolicity effects, the comparison with our calculation is, however, not straightforward. Recent cyclotron-resonance experiments with a 22-Å quantum well[15] will be discussed in a future article[12] where nonparabolicity effects in the barriers are estimated. When these effects are neglected the results are not expected to be accurate for well widths below 50 Å.

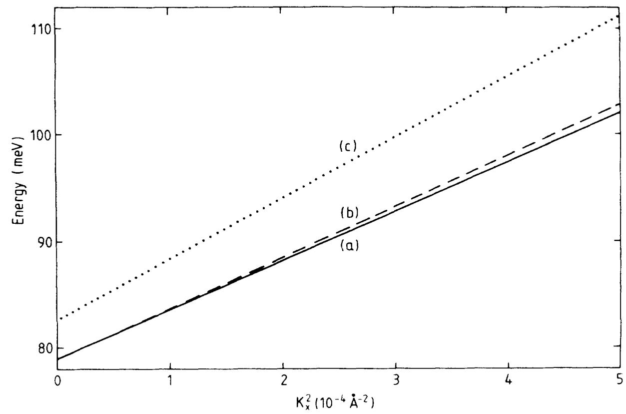

FIG. 1. Energy vs k^2 in the [100] direction for the ground state in a 50-Å-wide GaAs quantum well between $Al_{0.4}Ga_{0.6}As$ barriers. The solid line (*a*) shows the result of a numerical calculation while the dashed line (*b*) shows the result with the approximate first-order perturbation theory expression Eq. (20). For comparison we show the result when nonparabolicity effects are ignored [dotted line, (*c*)].

In conclusion, we have calculated the dispersion parallel to the layers of the electron subbands in a GaAs quantum well. Nonparabolicity effects have been taken into account using an expression with the bulk conduction-band dispersion expanded to fourth order in k. The anisotropy of the conduction band has been included but the spin splitting has been neglected. We find that the parallel mass, which is of importance for transport properties along the quantum well and for the density of states, is enhanced over the band-edge mass 0.0665 at least 3 times more than the perpendicular mass, which determines how the nonparabolicity influences the confinement energies. We have given some simple but accurate analytical expressions for the

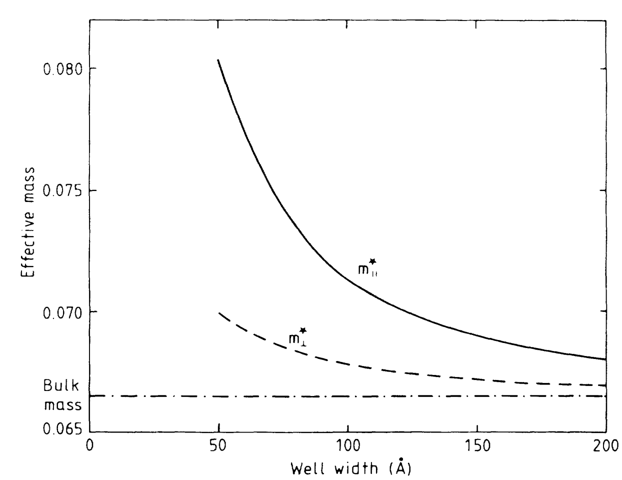

FIG. 2. Well-width dependence of the parallel effective mass defined by Eq. (18) (solid line) and the perpendicular mass defined by Eq. (10) (dashed line) (in units of the free-electron mass).

two masses. They explicitly depend on the confinement energy, which is experimentally accessible.

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[9]This is not the only way to define an energy-dependent effective mass, but it is the appropriate mass to use when the confinement energies are determined. The definitions $m^*=\hbar^{-2}d^2E/dk^2$ and $m^*=\hbar eB/\Delta E$ (cyclotron mass) give results different from ours in the nonparabolic case.

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