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Band nonparabolicity effects in semiconductor quantum wells

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We propose an empirical two-band model for heterostructures which provides a consistent energy-dependent effective-mass characterization of nonparabolicity in quantum wells. We show that it predicts several surprising results. Nonparabolicity has a very small effect on the lowest subband edge regardless of the well width and hence the energy of the state. Nonparabolicity causes a raising of the lowest subband edge rather than the expected lowering. Nonparabolicity causes a lowering of subband edge energies of higher subbands and the effect becomes substantial for the highest subband edges. We show that a large nonparabolicity lowering of a subband edge requires the state to have both a high-energy and a high occupancy probability in the well, i.e., not in the barriers.

Nonparabolicity in the neighborhood of energy-band extrema in bulk semiconductors can be described by the dispersion relation

$$E=\frac{\hbar^2k^2}{2m^*}(1-\gamma k^2)\ , \tag{1}$$

where E, k, and m^* are the energy, wave number, and effective mass of the charge carrier and γ is the nonparabolicity parameter. When a square quantum well is formed, for example, by a $Al_xGa_{1-x}As/GaAs/Al_xGa_{1-x}As$ ($x=0.37$) layered structure with a very narrow GaAs layer having a thickness of, say, 5 Å, the first (and only) electron subband edge calculated for a parabolic band has an energy of 265 meV and a wave number in the well of $6.8\times10^8\ m^{-1}$. Thus, from Eq. (1) the nonparabolicity term would be expected to cause a lowering of the edge by a fractional amount of order $\gamma k^2\sim0.23$ using $\gamma=4.9\times10^{-19}\ m^2$. This illustrates the importance of accounting correctly for nonparabolicity in analyzing phenomena in narrow quantum wells[1] or in higher lying subband edges in wider wells.

Recently, Hiroshima and Lang[2] argued that nonparabolicity in quantum wells is properly characterized by Eq. (1) along with both the interface boundary conditions and the barrier material dispersion relation lacking any dependence on nonparabolicity. In so doing they reject an alternative model in which the effective mass is energy dependent.

We believe the contrary to be true. We believe the best and most basic handling of nonparabolicity in quantum-well structures is contained in the Bastard derivation[3,4] of the envelope function approximation leading to a two-band (Kane) model. Further, we find that the equations resulting from this model can be recast into an energy-dependent effective-mass form in which the interface boundary conditions are obtained in a manner consistent with the nonparabolicity of the well and barrier material, and in which the correct effective masses can be entered as empirical parameters.

We also wish to show by numerical calculations that the empirical two-band model reveals several surprises: (1) there is almost no nonparabolicity effect on the lowest subband edge in quantum wells for all well widths; (2) the small nonparabolicity effect on the lowest subband edge causes an increase in its energy rather than the expected decrease (at least for parameters characteristic of the $Al_xGa_{1-x}As$-GaAs system); and (3) in wider wells the nonparabolicity effect reverses sign for higher subband edges, causing a lowering of the subband edge energy, and for the highest subband edges becomes substantial in size.

The Bastard treatment[3,4] considers the interaction of the conduction band and light-hole valence band in both the well and barrier materials at once throughout the heterostructure. The heavy-hole valence band does not interact with these bands and possesses only a small nonparabolicity from interaction with other bands. The interband interaction produces the same effective mass m^* characterizing the parabolic response of each band and the same γ parameter characterizing the nonparabolicity of each band. When cast into an energy-dependent effective-mass form, this model applied to just one of the bands for a single quantum square well consists of the dispersion relation in the well

$$E=\frac{\hbar^2k_w^2}{2m_w^*(E)}\ , \tag{2}$$

the dispersion relation in the barrier

$$E=V-\frac{\hbar^2k_b^2}{2m_b^*(E)}\ , \tag{3}$$

and the boundary condition

$$\left[\frac{k_wm_b^*(E)}{k_bm_w^*(E)}-\frac{k_bm_w^*(E)}{k_wm_b^*(E)}\right]\tan k_wl=2\ . \tag{4}$$

Here the subscripts w and b denote well and barrier, the wave numbers k_w and k_b are both real numbers corresponding to trigonometric wave functions in the well and exponentially decaying wave functions in the barriers, l is the well width, V is the energy barrier height at the interfaces, and the energy-dependent effective masses are given

by

$$m_w^*(E) \equiv m_w^*(1+E/E_w) \ , \tag{5}$$

$$m_b^*(E) \equiv m_b^*[1-(V-E)/E_b] \ , \tag{6}$$

where E_w and E_b are the energy gaps between the conduction and light-hole valence bands in the well and barrier materials. The nonparabolicity parameter is related to the energy gap and the effective mass by

$$\gamma_i = \frac{\hbar^2}{2m_i^* E_i}, \ (i=w,b) \ . \tag{7}$$

The model also relates these properties on the two sides of the interface by

$$m_w^*/m_b^* = E_w/E_b \ , \tag{8}$$

$$\gamma_w/\gamma_b = (m_b^*/m_w^*)^2 \ . \tag{9}$$

While the Bastard two-band model does represent a unified treatment of band properties in superlattice materials, it is unsuitable in its original form for application to real heterostructures since the effective masses and the nonparabolicity parameters are equal in this model for electrons and light holes in a particular material (well or barrier). However, it is well known, for example, that the effective masses of electrons and light holes in GaAs differ. Furthermore, it is not possible in this model to assign the experimental effective masses for both sides of the heterointerface. These differences along with a difference in the nonparabolicity parameters of electrons and light holes is caused by interactions with other, more distant (in energy) bands not included in the Bastard two-band model. In other words, inclusion of only two bands unduly restricts the parameter values of the model when interpreted literally.

For this reason we wish to modify the interpretation of the Bastard model. We regard the energy gap in Eqs. (5)–(8), when considering electrons, for example, as being an effective gap representing the appropriately weighted energy position of the combination of all bands interacting with the lowest (zone center) conduction band. Similarly, when considering light holes, we regard the energy gap as being an effective gap representing the appropriately weighted energy position of the combination of all bands interacting with the highest (zone center) light-hole valence band. Thus, we allow different gaps, different masses, and different nonparabolicities to be used for light holes and for electrons. We set the effective mass of either of the carriers to its experimental value for the well and determine by Eq. (7) the effective gap of the well for that carrier by using either an experimental value of γ for the well (if available) or the best available calculated value. We set the effective mass of the carrier to its experimental value for the barrier also and then determine the effective gap in the barrier from Eq. (8) and the nonparabolicity in the barrier from Eq. (9). Thus, in the empirical two-band model m_w, m_b, and γ_w are adjustable parameters.

In summary, we believe that the Bastard two-band treatment contains the correct basic physics of nonparabolicity, that it thus produces the essential functional dependences on this property in the dispersion relations and the boundary condition, and that our modified interpretation of Eqs. (5), (6), and (7) should bring it into closer conformity with experiment.

These views are supported by a comparison of Bastard's three-band model[5] of superlattices to his two-band model. In the three-band model the split-off valence band is added to the two-band model. In the three-band model the electron and light-hole masses become different, being related by $m_{\rm lh}^* = (\frac{3}{2})m_e^*(E_i+2\Delta_i/3)/(E_i+\Delta_i)$, $(i=w,b)$, where Δ_i is the energy splitting between the light-hole and split-off valence bands. We find that the three-band model can also be recast into the energy-dependent effective-mass formulation, Eqs. (2)–(4), and that for the $Al_xGa_{1-x}As$-GaAs system the masses can be approximated to an accuracy of better than 1:300 over the range of interest by

$$m_w^*(E) = m_w^*[1+E/(E_w+\Delta_w/3)] \ , \tag{10}$$

$$m_b^*(E) = m_b^*[1-(V-E)/(E_b+\Delta_b/3)] \ , \tag{11}$$

which can be seen to be identical with Eqs. (5) and (6) except for the energy gap replacement $E_i \rightarrow E_i+\Delta_i/3$ $(i=w,b)$. Also, it can be shown at this level of accuracy that Eqs. (7) and (8) continue to hold but with the same energy gap replacements, and that Eq. (9) retains its same form. Since we are treating the energy gap as an adjustable parameter in our interpretation of the Bastard model, the gap replacements just mentioned make no essential change in the energy-dependent effective-mass formulation of nonparabolicity.

It is worth noting that the empirical two-band model of nonparabolicity can be applied to any band minimum or maximum such as the heavy-hole or split-off valence bands. The small value of the nonparabolicity of the heavy hole would be reflected in large effective gaps E_w and E_b.

We calculated the subband edges for electrons in single square quantum wells of $Al_xGa_{1-x}As$/GaAs/$Al_xGa_{1-x}As$ ($x=0.37$) of various widths by Eqs. (2)–(9) and compared the results with those obtained when Eqs. (5) and (6) are replaced by constant masses, that is, results having no nonparabolicity.

We consider a conduction band with the interface energy barrier $V=f\Delta G$, where ΔG is the difference of energy gaps between barrier and well material taken as $\Delta G = 1.425x - 0.9x^2 + 1.1x^3$ (Ref. 6) and $f=0.6$ (Ref. 7). We take the electron effective mass in the GaAs well material as $0.0665m_0$. In the absence of an experimental value of the electron mass in the alloy material of the barrier, we interpolate its value between those of GaAs and AlAs ($0.15m_0$) using the spirit of Eq. (8), that is, that masses are proportional to energy gaps:[8] $m_e(x)/m_0 = 0.0665 + 0.0835\Delta G/1.625$. We use $\gamma = 4.9 \times 10^{-19}$ m^2 calculated with a five-band bulk-crystal model[9] for electrons in GaAs. Equation (9) then determines the γ value in the alloy material barrier.

Since the nonparabolicity might be expected to cause the largest effect, a lowering, on the subband edges when at a large energy in the well, we first calculate for a very narrow well of 5-Å width where the first and only subband edge is near the top of the well. We find its energy to be

265.27 meV with no nonparabolicity and 265.25 meV with no parabolicity. Surprisingly, the effect of nonparabolicity is not only minute but causes a raising, not the expected lowering, of the subband edge in this case.

A graphical representation of the solutions with and without nonparabolicity helps interpretation of the solutions. In Figs. 1(a) and 1(b) we exhibit E vs $k_w l/2$ and E vs $k_b l/2$ for the well width $l=5$ Å with and without nonparabolicity. From Fig. 1(a) it is apparent that the wave number in the well does change when nonparabolicity is added to the model, but that compensating changes occur in the combination of the dispersion relation in the barrier and the boundary conditions to diminish greatly the expected eigenenergy change. From Fig. 1(b) we see that k_b is small and changes only minutely with the addition of nonparabolicity. The smallness of k_b means not only a small nonparabolicity contribution from the two barrier regions but also a sizeable probability of the electron being in the barrier regions.

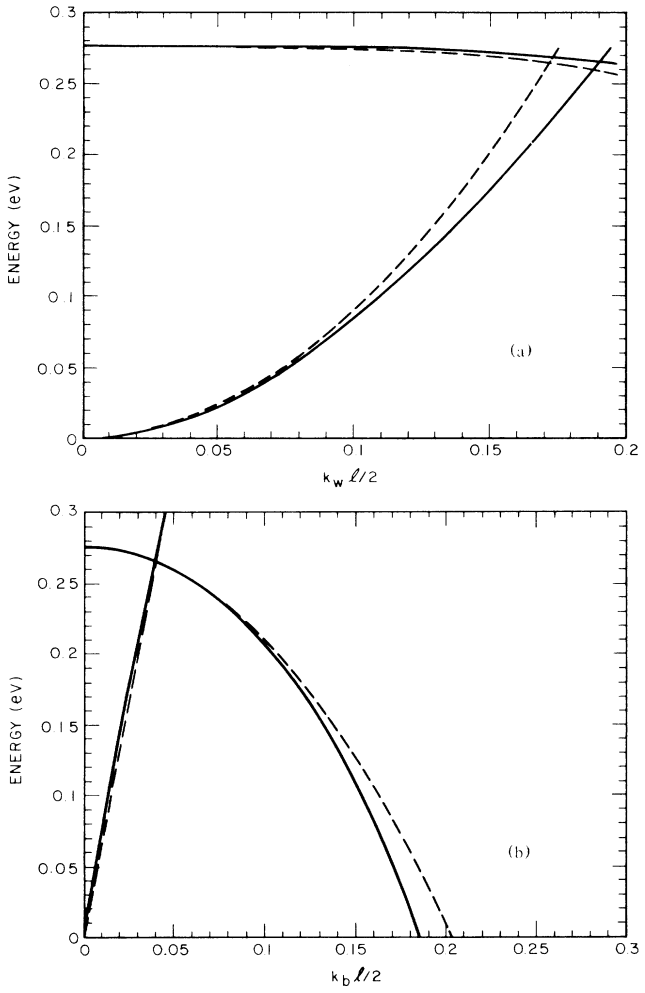

FIG. 1. (a) Eigenenergy determination for a 5-Å-wide square quantum well. Equation (2) and a combination of Eqs. (3) and (4) are plotted as energy vs well wave number k_w (normalized by one-half the well width $l/2$). Their intersection gives the eigenenergy of the state. Solid lines contain nonparabolicity, dashed lines do not. (b) Equation (3) and a combination of Eqs. (2) and (4) are plotted as energy vs barrier wave number k_b (normalized by one-half the well width $l/2$).

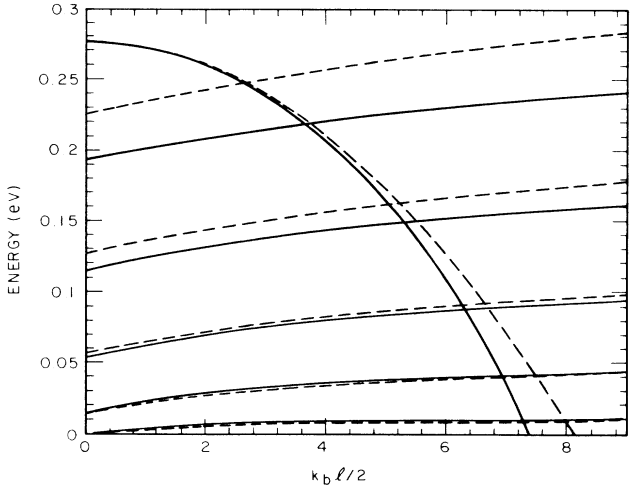

FIG. 2. Same as Fig. 1(b) except $l=200$ Å.

A plot of E vs $k_b l/2$ for a well width of 200 Å is shown in Fig. 2. Five bound states of the well occur for this well width. The nonparabolicity effect is again seen to be minute for the lowest state and to grow in size for the higher states. The minute effect on the lowest state results from a small eigenenergy and small well wave number. The highest state, which, however, has a lower energy than the one state in the 5-Å well, has a large nonparabolicity effect. Note also how the curves with and without nonparabolicity cross over as the quantum number increases.

In Table I we list salient characteristics of the eigensolutions illustrated in Figs. 1 and 2 and those for three intermediate well widths. There we list the subband edge energy E, the energy shift E_{np} due to nonparabolicity

TABLE I. Well width and associated eigenstate energies, energy shifts from nonparabolicity, and well occupancy probability versus quantum number n of the eigenstate.

l (Å)		n = 1	2	3	4	5
5	E (meV)	265.27				
	E_{np} (meV)	+0.02				
	O_w	0.075				
20	E	180.90				
	E_{np}	+1.01				
	O_w	0.546				
50	E	81.17	254.67			
	E_{np}	+1.47	−13.87			
	O_w	0.881	0.405			
100	E	32.30	119.52	235.79		
	E_{np}	+0.70	−4.84	−22.87		
	O_w	0.972	0.884	0.658		
200	E	10.55	41.11	88.82	149.74	218.93
	E_{np}	+0.19	−0.25	−3.81	−13.21	−28.22
	O_w	0.995	0.980	0.953	0.910	0.825

measured from a parabolic dispersion solution, and the probability of occupancy O_w in the well (as distinct from the barriers) for the eigenstate.

These data for quantum wells illustrate the unexpected dependence on nonparabolicity. First, we see that the lowest subband edge has a very small shift due to nonparabolicity regardless of well width and hence of how high in energy it is above the conduction band edge in the well. Second, the effect of nonparabolicity on the lowest subband edge causes a *raising* of the subband edge, rather than the expected lowering for the well width. Third, the nonparabolicity shift becomes the expected lowering for higher subband edges when they exist in wider wells. Fourth, the nonparabolicity shift becomes substantial for the highest subband edge for well widths $\gtrsim 100$ Å.

The clearest dependence of the energy shift from nonparabolicity is on the quantum number of the subband edge: a small (large) quantum number causing a small (large) nonparabolicity effect. This can be understood by a consideration of the energy of the state and the wave number and occupancy probability values in the well and in the barriers. Consider the one state in the 5-Å well. It has a high energy and thus a high wave number in the well which implies a large nonparabolicity effect in the well. However, the electron spends only 7.5% of the time in well. The other 92.5% of the time is spent in the barriers where, as seen from Fig. 1(b), the wave number and hence the nonparabolicity effect are small. Consider for contrast the highest state in the 200-Å well. There the energy and the wave number in the well are high with a consequent large nonparabolicity effect. In contrast to the 5-Å well the occupancy probability in the well is 82.5% for the 200-Å well, thus allowing the full expression of the nonparabolicity. We conclude that high quantum-number states have large nonparabolicity effects because they have both large energies and large well occupancy probabilities. We can also conclude that the barrier regions never make a large contribution to the nonparabolicity of a quantum-well state because, when the wave number in the barrier is high (low) leading to high (low) nonparabolicity in the barriers, the occupancy in the barriers is low (high).

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