Quasistationary-energy-level calculation for thin double-barrier
GaAs-Ga_{1-x}Al_x As heterostructures

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A band-structure calculation for thin double-barrier GaAs-Ga_{1-x}Al_x As heterostructures is
developed by identifying quasistationary energy levels with resonances in the transmission
coefficient, which is obtained with the transfer-matrix technique. The results are compared with
calculations for isolated quantum wells and superlattices. Exact numerical calculations for the
broadening and the shift of energy levels with decreasing barrier width are presented. Changes in
the curvature of the band structure are found. An approximate formula for the energy levels and
widths of the quasistationary states of double-barrier systems is developed. The formalism is based
on a Fano-type configuration interaction between the eigenstates of appropriate subsystems.

I. INTRODUCTION

The electronic structure of isolated quantum wells
(QW's) or superlattices (SL's) has been the subject of
several theoretical studies for which references are given
in Ref. 1. The envelope-function approximation
turned out to be an effective method to calculate the band
structure of these systems.

Isolated semiconductor QW's [Fig. 1(a)] are handled in
a similar manner as textbook potential wells; instead of
plane waves, the Bloch functions of the host semiconductor
are used. The stationary states (and corresponding
energy levels) are obtained by matching the linear com-
binations of the allowed bulk solutions at the potential
steps. Juxtaposing several QW structures, we obtain a SL
[Fig. 1(b)]. For a sufficiently large number of periods,
the Bloch theorem can be applied and the calculation of
the stationary states can be treated in a way similar to a
Kronig-Penney problem.2

A QW delimited by double barriers with finite width
[Fig. 1(c)] may, on the one hand, be seen as the lower lim-
it of a SL structure with few periods, or, on the other
hand, as a single QW which is no longer isolated. The
electronic states of the system are quasistationary with a
finite lifetime \( \tau \).

In this paper we present a band-structure calculation
for thin barrier heterostructures. The method is based on
the identification of the energy levels of the quasistation-
ary states with resonances in the transmission coefficient
\( D(E) \). To calculate the transmission coefficient, the
envelope-function approximation and the transfer-
matrix technique are applied. In the case of holes we use
an extension of the transfer-matrix technique to a
four-component Luttinger-Kohn wave function,11 as
presented in Ref. 12.

In Sec. II the formalism is described. Calculated band
structures for the case of Fig. 1(c) with thick barriers are
compared with the results for isolated QW's (Ref. 1) and
SL's.3 We show in Sec. III the energy \( E(k_z=0) \) of the
quasibound states as a function of barrier width, as well
as the in-plane band-structure \( E(k_z) \) for two different
barrier widths. For small barrier width the energy of the
quasibound states is shifted by several meV and the cur-
vature of the in-plane band structure changes drastically
for light-hole (LH) subbands. Experimental evidence of
these effects is sought by analyzing luminescence spectra
of QW's with different barrier widths.13

In Sec. IV we combine the Bardeen model for tunneling
with the Fano model for configuration interaction and
derive an approximate formula for the energy posi-
tion and widths of the quasistationary states of double-
barrier heterostructures. Finally, in Sec. V we summarize
results and conclusions.

FIG. 1. Typical band-edge profiles for GaAs-Al_xGa_{1-x}As heterostructures. (a) Isolated quantum well, (b) superlattice, (c) quantum well with finite-width barriers.

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II. METHOD OF CALCULATION

To calculate the transmission coefficient $D(E)$ for electrons we follow Refs. 7 and 8 using the effective-mass approximation and the transfer-matrix technique, taking into account the different effective masses in each layer.

The valence bands are described by the effective-mass Hamiltonian of Luttinger and Kohn. Neglecting the conduction bands and the spin-orbit-split bands, the effective-mass Hamiltonian is a $4 \times 4$ matrix operator $H$ which acts on a four-component envelope function. Exact solutions for the effective-mass equation in the bulk were recently given. The transmission coefficient $D(E)$ for holes is derived by applying an extension of the transfer-matrix technique using the four-band effective-mass equation. This technique is described in Ref. 12 and only basic steps are reviewed here. In terms of the exact bulk solutions and the boundary conditions described in Ref. 1, and using the transfer-matrix technique for the four-component envelope function at each interface, we relate outgoing amplitudes $t$ to the incoming ones $a$ (Ref. 12)

$$t = Ma,$$  (1)

where $t$ and $a$ are now eight-component column vectors and the transfer matrix $M$ is $8 \times 8$. The transmission coefficient $D_j$ through channel $j$ is

$$D_j = |t_j|^2N,$$  (2)

where $N$ is a normalization factor.

The band structure $E(k_y)$ is derived by identifying the resonance energy $E_R$ of $D(E,k_y)$ with the quasibound energy level.

We compare the band-structure calculations for thick double-barrier heterostructures based on the transfer-matrix technique with the calculations for an isolated QW (Ref. 1) and a SL. For example, in the case of 100-Å barriers, (see Fig. 5 of Ref. 3), deviations occur only for the second LH subband, very close to the top of the barriers, since the corresponding wave functions in the barriers have a large decay length. A similar comparison with the calculation for a SL with 200-Å barriers (see Fig. 4 of Ref. 3) shows no differences between the two kinds of calculations.

III. EFFECT OF BARRIER WIDTH ON THE IN-PLANE BAND STRUCTURE

The effect of barrier width on the in-plane band structure can be calculated exactly by use of the transfer-matrix technique. In Fig. 2(a) we compare the in-plane band structure of equally wide QW's with two different barrier widths. The first two subbands (HH1, LH1) are shifted to smaller absolute energy as the barrier width decreases, while the (heavy-hole) HH2 subband is shifted to larger absolute energy. Most interestingly, the curvature of the in-plane band structure changes drastically. As an example for the broadening of the energy level, in Fig. 2(b) the transmission coefficient $D(E)$ in the energy region of the HH1 subband with $k_y = 0$ is shown for the two barrier widths. As seen in Fig. 3, effects of the barrier width $b$ become important for $b < 30$ Å.

The shift in binding energy by the barrier width should be observable in resonant tunneling or luminescence measurements. Recently, Tsuchiya et al. measured luminescence spectra of nonisolated quantum wells for different barrier width in the range from 28 to 62 Å. The spectrum of the 28-Å sample is shifted to smaller energy by about 3 meV in comparison to the 62-Å sample. This

![Figure 2](image-url)
IV. ENERGY LEVELS OF QUASISTATIONARY STATES IN QUANTUM WELLS WITH FINITE BARRIERS

For a qualitative understanding of the exact numerical results in Sec. III, derived by a matching procedure, we discuss in general the energy levels and widths of quasistationary states in quantum wells with finite barriers. Let $H_0$ be a Hamiltonian with a continuous spectrum $|\nu\rangle$ and a discrete spectrum $|n\rangle$ of stationary states with energy eigenvalues in the same energy range. An additional constant perturbation $V$ causes transitions from the discrete states into the continuum. The transition-matrix element $\langle \nu | V | n \rangle$ broadens and shifts the formerly discrete energy levels. It should be noticed that $|\nu\rangle$ and $|n\rangle$ are the eigenstates of the unperturbed Hamiltonian $H_0$. Energy-level shift and broadening can be calculated by either time-independent\(^{16}\) or time-dependent\(^{17}\) perturbation theory. Fano\(^{15}\) derives a nonperturbative calculation for the level shift and broadening starting from the matrix of the perturbed Hamiltonian $H = H_0 + V$ in the basis of the eigenstates $|n\rangle$ and $|\nu\rangle$ of $H_0$. To calculate the level shift and broadening for the quantum well [Fig. 5(a)] when it goes over to a well with finite barriers [Fig. 5(d)], neither of the above formalisms can be applied. There is no term in $H$ which is small (as required for perturbation theory) and it is not obvious how to write an $H_0$ with continuous states degenerate with a discrete level (as required for a Fano formalism).

Bardeen\(^{14}\) calculates tunneling through a barrier by using eigenstates of appropriate subsystems $H_i$. These eigenstates of $H_i$ are approximate solutions of the exact Hamiltonian $H$. We combine this idea with the Fano formalism\(^{15}\) to give an approximate formula for energy levels and widths of a quantum well with finite barriers. The subsystems $H_i$ are defined by Figs. 5(a), 5(b), and 5(c), and the exact Hamiltonian $H$ is defined by Fig. 5(d). The eigenvalue equations of these different systems are

![Energy levels of a nonisolated quantum well](image1)

**FIG. 3.** Energy levels of a nonisolated quantum well at $k_{||} = 0$ as a function of barrier width $b$ ($L = 50$ Å, $V_0 = -95.65$ meV, $x = 0.21$, (10)).

![Conduction in-plane band structure](image2)

**FIG. 4.** Conduction in-plane band structure of a nonisolated quantum well for two different barrier widths $b = 100$ Å (solid line), $b = 10$ Å (dashed line) ($L = 50$ Å, conduction-band offset $V_0 = 143.48$ meV, $x = 0.21$).

![Subsystems](image3)

**FIG. 5.** Subsystems for a quantum well with finite-width barriers. (a) $H_0$, isolated quantum well; (b) and (c) $H_1$ and $H_2$, potential steps; (d) $H$, double-barrier heterostructure.
TABLE I. Comparison of the $\Gamma$ values derived from the matching procedure $\Gamma_m$ and from the Fano-like formalism (7) $\Gamma_F$ (barrier height $V_0$, well width $L$, barrier width $b$).

<table>
<thead>
<tr>
<th>$V_0$ (eV)</th>
<th>0.1</th>
<th>0.1</th>
<th>0.1</th>
<th>0.5</th>
<th>0.5</th>
<th>0.5</th>
<th>0.1</th>
<th>0.1</th>
<th>0.1</th>
<th>0.1</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$ (Å)</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>100</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>$b$ (Å)</td>
<td>30</td>
<td>50</td>
<td>80</td>
<td>30</td>
<td>50</td>
<td>70</td>
<td>30</td>
<td>50</td>
<td>80</td>
<td>100</td>
</tr>
<tr>
<td>$\Gamma_m$ (meV)</td>
<td>5.3</td>
<td>1.2</td>
<td>0.1</td>
<td>0.1</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.8</td>
<td>0.1</td>
<td>0.01</td>
<td>&lt;0.01</td>
</tr>
<tr>
<td>$\Gamma_F$ (meV)</td>
<td>4.5</td>
<td>1.1</td>
<td>0.1</td>
<td>0.1</td>
<td>&lt;0.01</td>
<td>&lt;0.01</td>
<td>0.4</td>
<td>0.1</td>
<td>0.01</td>
<td>&lt;0.01</td>
</tr>
</tbody>
</table>

\begin{align}
H_0 | \psi \rangle &= \varepsilon_n | \psi \rangle, \\
H_1 | \psi \rangle &= \varepsilon | \psi \rangle, \\
H_2 | \chi \rangle &= \varepsilon | \chi \rangle, \\
H | \phi \rangle &= \delta | \phi \rangle. \\
\end{align}

The Hamiltonian matrix of $H$ in the eigenstates $| \psi \rangle, | \psi \rangle, | \chi \rangle$ of the subsystems $H_0, H_1, H_2$ is

\begin{align}
\langle \phi | H | \psi \rangle &= E_\psi, \\
\langle \phi | H | \psi \rangle &= V_\psi \varepsilon \langle \chi | H | \psi \rangle = W_\psi \varepsilon; \\
\langle \phi | H | \psi \rangle &= \varepsilon \delta (\varepsilon - \varepsilon); \\
\langle \phi | H | \chi \rangle &= 0.
\end{align}

where in (4c) terms of the order $\varepsilon_0 / V_0$ and in (4d) terms of order $e^{-2L} \kappa = [(2m / \hbar^2)(V_0 - \varepsilon)]^{1/2}$ are neglected. While the eigenstates of each subsystem are orthonormal, it is important to notice that the overlap integrals are not zero:

\begin{align}
\langle \psi | \psi \rangle \neq 0, \\
\langle \phi | \chi \rangle \neq 0,
\end{align}

since $| \psi \rangle, | \psi \rangle, | \chi \rangle$ are eigenstates of different Hamiltonians. For large $L$ [see Fig. 5 (d)], $\langle \psi \varepsilon | \chi \rangle$ is approximately zero to order $e^{-2L}$. The eigenstates $| \phi \rangle$ of $H$ are expanded in the eigenstates of the subsystems

\begin{align}
| \phi \rangle &= \alpha | \phi \rangle + \int d \varepsilon (b_\varepsilon | \psi \rangle + c_\varepsilon | \chi \rangle)
\end{align}

and a procedure similar to that shown in Ref. 15 but with use of Eq. (5) gives

\begin{align}
E_\phi &= \int d \varepsilon \left( V_\varepsilon - E \langle \psi | \phi \rangle \right)^2 + \left| W_\varepsilon - E \langle \chi | \phi \rangle \right|^2 \\
&= \frac{-i \pi}{E - \varepsilon} \int d \varepsilon \delta (E - \varepsilon) (V_\varepsilon - E \langle \psi | \phi \rangle)^2 + \left| W_\varepsilon - E \langle \chi | \phi \rangle \right|^2 = E.
\end{align}

If the overlap integrals are zero, Eq. (7) is formally identical to the results in Sec. IV of Ref. 15, but nevertheless it is different since in (7) the matrix elements are calculated with the eigenstates of the subsystems and not with the eigenstates of the unperturbed Hamiltonian as in Ref. 15.

The solution of (7) is the complex energy $E = E_0 - \frac{1}{2} i \Gamma$ of the quasibound energy level, where the imaginary part expresses the decay $e^{-\Gamma t / \hbar}$ of probability density in the well and $\Gamma$ is the halfwidth.\(^{16}\) For a demonstration of the validity of the formalism we calculate the $\Gamma$ from (7) and compare it (Table I) with the $\Gamma_m$ derived from the full width at half maximum of the transmission resonance obtained by the matching procedure, for several typical cases. Both values are in all cases of the same order and for large barriers the values are in reasonable agreement, taking into account the approximations involved in Eqs. (4)–(6) and discussed above.

V. SUMMARY AND CONCLUSIONS

We presented a band-structure-calculation formalism for thin double-barrier GaAs-Ga1-xAlxAs heterostructures applying an extension of the transfer matrix technique\(^{12}\) to the envelope functions. The results for a QW with barriers of finite width are compared with former calculations for isolated QW’s (Ref. 1) and SL’s.\(^{3}\) In this comparison, QW’s with 100 Å barriers show only small deviations at large absolute energy. Decreasing the barrier width to 10 Å affects the in-plane band structure drastically. Energy shifts up to 8 meV in both directions occur and the curvature changes, most strongly for LH subbands. These results agree qualitatively with a recently observed shift in luminescence spectra for different barrier width.\(^{13}\) A general formalism to calculate approximately the energy levels of quasistationary states in quantum wells with finite barriers is presented. The formalism uses eigenstates of approximate subsystems.


\(^{4}\)J. C. Maan, in Magnetic Quantization in Superlattices, Vol. 27
of Festkörperprobleme (Advances in Solid State Physics), edited by P. Grosse (Pergamon/Vieweg, Braunschweig, 1987), p. 137. Figure 10 and text contain an instructive discussion on behavior of magnetic energy levels by the evolution from a single quantum well to a superlattice.


J. J. Sakurai, Modern Quantum Mechanics (Benjamin/Cummings, New York, 1985), Sec. 5.8.