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The consequences of a highly nonparabolic band structure on intersubband resonance are explored with experiments and theory on InAs/AlSb quantum wells. From a single-particle viewpoint, the intersubband resonance is expected to be broad because the intersubband spacing is highly k -dependent. Experimentally, however, we observe a relatively narrow line and this is interpreted as evidence that the intersubband resonance corresponds to a collective response of the high density electron system. Calculations taking into account resonant screening reproduce the experimental results reasonably well. Band nonparabolicity is shown from $\mathbf{k} \cdot \mathbf{p}$ theory to have no marked effects on the intersubband matrix elements both for conventional perpendicular excitation and for parallel excitation where the matrix elements, although non-zero, are small. These results are confirmed experimentally by tilting the sample with respect to the light beam.

1. Introduction

The consequences of electron–electron interactions on intersubband resonance have been studied for some considerable time [1]. For GaAs systems there are two fundamental effects, the resonant screening of the light (alternatively called the depolarization field) which increases the resonance energy, and the exciton interaction whereby an excited electron interacts with the hole in the Fermi sea it leaves behind tending to decrease the resonance energy [2]. The depolarization field, as calculated in a one-band approximation, does not change the linewidth.

The focus of the present work is to explore the consequences of conduction band nonparabolicity on the intersubband resonance, in particular on the linewidth. The most immediate consequence of nonparabolicity is that the single-particle transition energy at the band minimum $k=0$ is higher than that at the Fermi wave vector $k=k_f$. This difference is naturally small in a modestly doped GaAs system, but it can be very large, some tens of meV, in a highly doped narrow gap system. Our experiments show that in such a system the intersubband resonance does not have the single-particle broadening; the line is relatively narrow. The explanation lies in the depolarization field: resonant screening is shown to lead to a collapse of the single-particle broadening. In this sense

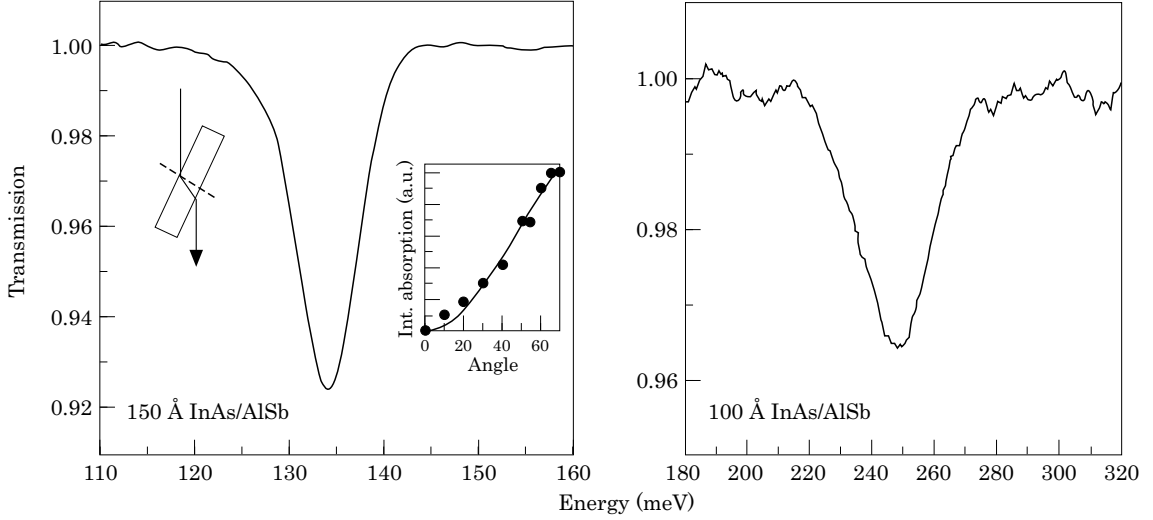


Fig. 1. Experimental spectra of InAs/AlSb multi-quantum wells taken in the Brewster angle geometry at 4 K. The inset shows absorption against incident angle, and the line is $E_z^2 \propto \cos^2 \theta / \sin \theta$ where θ is the angle to the normal in the sample.

the resonance we measure is a collective effect. The results are not complicated by the exciton because it is relatively unimportant in a narrow band system where the effective mass, and hence density of states, is small.

Results are presented here on InAs/AlSb quantum wells which are highly suited to the present study for three reasons. First, InAs is a narrow gap semiconductor and as such has a highly non-parabolic conduction band dispersion. Secondly, the quantum well barriers are very high so that very high carrier densities can be achieved, up to $5 \times 10^{12} \text{ cm}^{-2}$, and hence very high Fermi wave vectors. Finally, with MBE growth samples of very high quality are available so that the inhomogeneous broadening is minimized. The linewidth is first considered and shown to be narrow in relation to the single-particle broadening. Calculations of resonant screening are then shown to account for the experimental data reasonably well. Finally, the influence of nonparabolicity on the intersubband matrix elements is also considered. This has been a somewhat controversial subject recently, with several groups claiming either from theory [3–5] or from experiment [6–9] that nonparabolicity allows the intersubband resonance to be excited with in-plane polarization. This goes against conventional wisdom which asserts that the polarization must lie perpendicular to the quantum well plane, i.e. along the direction of confinement. We argue against a strong excitation of intersubband resonance with in-plane polarization, and this is confirmed with experiments on our InAs quantum wells by progressively tilting the sample with respect to the light beam.

2. Techniques

2.1 Experiments

We present intersubband resonance on two InAs/AlSb multi-quantum well samples grown by MBE. The samples have 20 wells, with thicknesses 100 and 150 Å, and carrier concentrations N_s of 3.0 and $2.5 \times 10^{12} \text{ cm}^{-2}$, respectively. We excited intersubband resonance by holding the sample close to the Brewster angle which gives a small component of electric field in the growth direction. The advantage

of this method is that it is possible to estimate the electric field in the sample and also to change it controllably simply by tilting the sample. Spectroscopy was carried out with a Fourier transform spectrometer with the samples either at 4 K or at room temperature and reference spectra were taken either from a substrate or from another InAs/AlSb sample. Spectra for the two samples are shown in Fig. 1 with resonances corresponding to wavelengths of about 5 and 9 μm . The resonances are reasonably symmetric in shape, somewhere in between Gaussian and Lorentzian in form, and narrow, the full width at half maximum (FWHM) for the 150 Å sample is 6.6 meV for instance. We also recorded spectra with the sample perpendicular to the light beam but we observed no resonances in this geometry. Finally, we measured the absorption strength as a function of incident angle at room temperature (where we have good control of polarization and angle); these results will be discussed below.

2.2 Band structure

We have accounted for band nonparabolicity in the InAs conduction band with $\mathbf{k} \cdot \mathbf{p}$ theory in which the wave function is expanded as

$$\psi(\mathbf{r}) = \sum_i \exp(i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel}) \phi_i(z) |i\rangle \quad (1)$$

where the $|i\rangle$ are the Bloch functions, varying rapidly on the atomic scale, the ϕ_i are the envelope functions, varying on the scale of the quantum well potential, and $\exp(i\mathbf{k}_{\parallel} \cdot \mathbf{r}_{\parallel})$ simply expresses plane wave motion in the plane. The growth direction is taken to be z and we consider just the x direction in the plane. The ϕ_i s are related to each other by an effective Hamiltonian where off-diagonal matrix elements imply coupling between the s - and p -like Bloch functions. We have taken the Kane [10] form of the Hamiltonian which reproduces conduction band nonparabolicity accurately, as can be judged from cyclotron resonance experiments [11].

The solutions are either $s\uparrow$ or $s\downarrow$ but with admixtures of p -like valence band states. The energy eigenvalues can be determined by setting one of the s -state ϕ s to zero and systematically eliminating all the other components. We then find that the $\mathbf{k} \cdot \mathbf{p}$ theory yields a simple Schrödinger equation

$$\left(-\frac{\hbar^2}{2m^*m_0} k_x^2 - k_z \frac{\hbar^2}{2m^*m_0} k_z + E_g(z) - \delta(z) \right) \phi_1 = E \phi_1, \quad (2)$$

but with a position and energy dependent mass:

$$\frac{1}{m^*(z,E)} = \frac{E_p}{3} \left(\frac{2}{E + \delta(z)} + \frac{1}{E + \Delta(z) + \delta(z)} \right). \quad (3)$$

E , E_g , Δ , E_p , and δ are the energy, fundamental band gap, spin-orbit splitting, Kane energy, and valence band offset, respectively.

The boundary conditions to eqn (2) were taken to be that ϕ_1 and $1/m^* \partial \phi_1 / \partial z$ are continuous at each interface. We also explored the case when $\phi_1 \rightarrow 0$ at the interfaces, strictly appropriate for an infinitely high potential well. Furthermore, we also solved eqn 2 when the effective masses are taken to be energy independent, 0.023 for the well and 0.117 for the barrier, to compare multi-band and one-band models.

The solutions for a 150 Å quantum well, using the parameters as listed in Table 1, are shown in Fig. 2. The importance of nonparabolicity is immediately apparent in that the energies are far from quadratically dependent on subband index and in that the dispersions as a function of k_x are obviously nonparabolic even at moderate k_x .

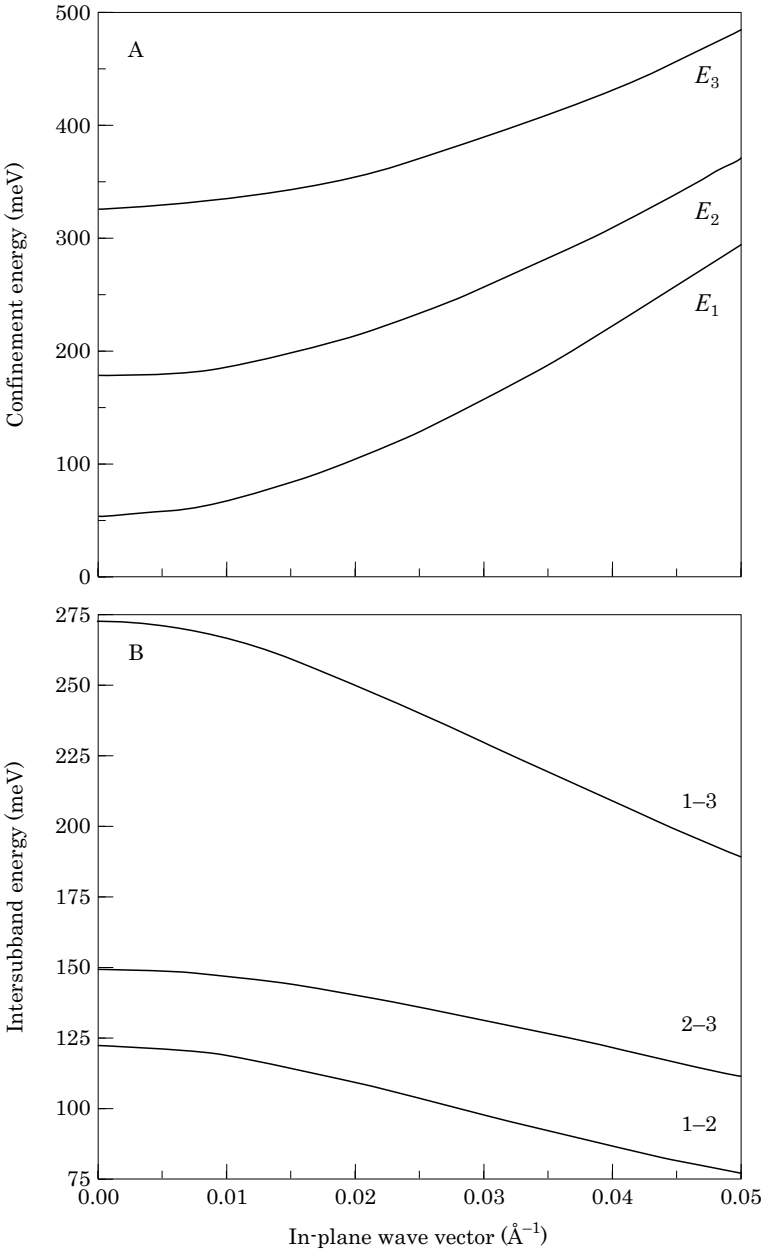


Fig. 2. A, The subband confinement energies, and B, the intersubband energies for a 150 Å InAs/AlSb quantum well.

3. The linewidth

One obvious effect of nonparabolicity is that the intersubband energy at $k=k_f$ is considerably smaller than that at $k=0$; for a 150 Å well we have 104.4 and 122.9 meV for a density $N_s=1 \times 10^{12} \text{ cm}^{-2}$. Nevertheless, the experimental spectrum is narrow on this energy scale. The explanation lies in the collective effects which obscure the single-particle spectrum.

Table 1: The parameters used in the calculations for InAs/AlSb structures

	InAs	AlSb
E_g (eV)	0.418	2.32
Δ (eV)	0.38	0.75
E_p (eV)	21.5	
δ (eV)	0.0	-0.198
ϵ_r	12.25	

It is well known that screening of the light field by a high density electron gas leads to an up-shift in the energy of the intersubband transition. In a one-band approximation [12], the lineshape is unaltered but the absorption occurs at an energy \tilde{E} where

$$\tilde{E}^2 = E_{12}^2 + E_{pl}^2 \quad (4)$$

E_{pl} is a plasma energy given by

$$E_{pl}^2 = \frac{2e^2 N_s S E_{12}}{\epsilon_o \epsilon_r} \quad (5)$$

and S is the depolarization integral

$$S = \int_{-\infty}^{\infty} \left[\int_{-\infty}^z \phi_2(z') \phi_1(z') dz' \right]^2 dz \quad (6)$$

What is less well known, however, is that the depolarization effect leads to a line-narrowing for a nonparabolic system [13].

To incorporate the depolarization effect into our theory we have extended the original time-dependent perturbation theory of Allen *et al.* [12] to cope with the multi-component wave function. For the real part of the conductivity we arrive at

$$\Re(\sigma_{zz}) = \frac{2e^2}{\hbar} \frac{N_s \langle z_{12} \rangle^2 E}{E_{12}(0)} \Im \left(\frac{G(E)}{1 + \frac{E_{pl}^2}{E_{12}(0)^2} G(E)} \right) \quad (7)$$

with

$$G(E) = \frac{1}{\pi N_s} \int_0^{k_f} \frac{k E_{12}(0)^2}{E_{12}(k)^2 - E^2 - iE\Gamma} dk \quad (8)$$

in agreement with Załuźny [13]. In these equations, E is the light energy, and Γ is an energy broadening of the levels. For an infinitely high quantum well in a one-band model the S -integral can be calculated analytically as $S = 5L/9\pi^2$, 8.44 Å for $L = 150$ Å. A calculation of S using the multi-component wave functions yields the remarkably similar 8.49 Å, and furthermore exhibits practically no k_x -dependence. We plot the lineshape for $S=0$ (i.e. without the depolarization) and for $S \neq 0$ for $\Gamma = 1$ and 5 meV in Fig. 3. The $\Gamma = 1$ meV traces make it clear that the main peak in $\Re(\sigma_{zz})$ has a width

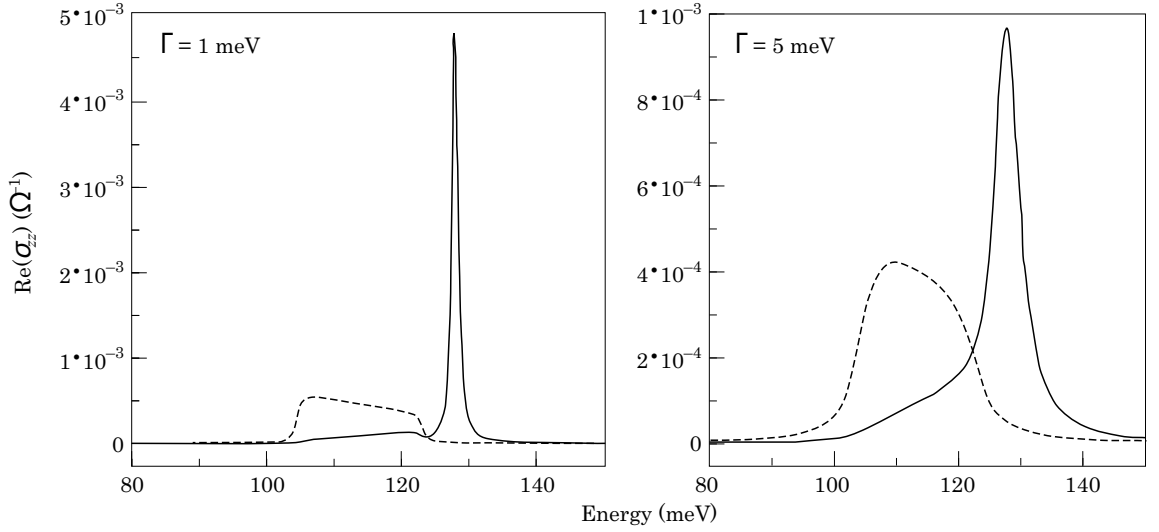


Fig. 3. The calculated real part of the conductivity for a 150 Å quantum well with carrier concentration $1 \times 10^{12} \text{ cm}^{-2}$. $S=0$ (dotted lines) neglects the depolarization field; $S \neq 0$ (solid lines) includes it, and results are given for values of the broadening parameter Γ , 1 and 5 meV.

determined not by the spread of the function $G(E)$ but simply by the line broadening Γ . Additionally, there is a weak absorption in the one-particle energy range, which evolves into a low energy tail at higher Γ . The integrated absorption is the same in both cases.

The experimental data of Fig. 1 for the 150 Å well verify that the depolarization field is playing an important role in that the linewidth is considerably narrower than the single-particle broadening. In fact, this broadening has been experimentally observed by exciting the intersubband resonance with an in-plane magnetic field which, in conjunction with crystal inversion-asymmetry, excites a spin-flip transition which is not influenced by the depolarization field [14]. Furthermore, the energy of the resonance, 134 meV, is substantially higher than even the calculated $k=0$ gap and this is also a consequence of the depolarization field as can be confirmed with the parallel magnetic field experiment.

The theory, essentially the random phase approximation (RPA), describes the experimental lineshape reasonably well. However, the experimental lineshape is not exactly Lorentzian and we have not seen any evidence for a low energy tail and these may be indications that terms beyond the RPA are influencing the resonance to some extent.

Another example of a broad single-particle spectrum is the absorption between the first two minibands in a superlattice. Simply from the Kronig-Penney dispersion it is clear that the transition energy at the minizone centre is larger than that at the minizone edge. Calculations for such a case have been performed [15,16] (also in the RPA) and yield spectra remarkably similar to those of Fig. 3; namely, there is a strong peak corresponding to a collective mode, termed an interminiband plasmon in Zhang *et al.* [15], and a broad response at lower energies corresponding to the single-particle transitions. As the miniband widths decrease the single-particle transitions gradually disappear so that ultimately all the oscillator strength resides in the depolarization shifted intersubband resonance. To the best of our knowledge, an interminiband plasmon has not been observed experimentally; instead, experiments seem to have been carried out in the other limit when the miniband widths are very large and single-particle effects dominate [17]. The general point would appear to be

that when the plasma energy is comparable to the energy gaps in the system a collective mode can be expected.

4. Energy and matrix elements

The energy of the intersubband resonance is clearly influenced by nonparabolicity: at $k=0$ for instance the single-particle 1–2 energy is 122.9 (141.9) meV with (without) nonparabolicity. However, in order to make detailed comparisons with the experiments we have the peculiarity that for the 150 Å well we do not observe the 2–3 transition although the carrier concentration is high enough for the second subband to be occupied. Assuming that the Fermi level lies just below the second subband ($N_s = 1.8 \times 10^{12} \text{ cm}^{-2}$) we calculated a depolarization-shifted energy of 132.7 meV which is in good agreement with the experiments. For the 100 Å well, the second subband cannot conceivably be occupied but our theory predicts 213 meV against the measured 248. The origin of this discrepancy is not clear, but we note that the alternative boundary conditions ($\phi \rightarrow 0$) give much better agreement, to within ~ 10 meV. More experiments on narrow wells are required to resolve this point.

The absorption A is related to the conductivity by

$$A = \frac{\Re(\sigma_{zz})}{\epsilon_0 c \sqrt{\epsilon_r}} \quad (9)$$

and so is proportional to $\langle z_{12} \rangle^2$. From the measured absorption we estimate $\langle z_{12} \rangle = 28 \pm 5$ and 23 ± 4 Å for the 150 and 100 Å samples, respectively. Exciting the intersubband resonance with an in-plane magnetic field gave 25.0 Å for the 150 Å well, and this is a more accurate method as it does not require a detailed knowledge of the electric field distribution in the sample [18].

In order to compute the matrix elements and therefore also selection rules we make the standard separation of the electric dipole integral [19]. The general point is that, in every case, transitions are allowed by interactions of the s -like component in one state with the p -like component in the other. In this sense, intersubband transitions are not fundamentally different from interband transitions [20]. A selection rule exists for a symmetric confining potential, namely that 1–2 excited with $x(z)$ polarization is spin flip (conserving) [3], but this gives no indication of the magnitudes of the matrix elements. In order to estimate the matrix elements we have taken $k_x = 0$ and assumed that the vast majority of the wave function lies in the well. For $M_{12}^x = \langle \psi^1 | k_x | \psi^2 \rangle$ the four integrals add and we have

$$\frac{E_p}{6} \left[\frac{2}{E_1} + \frac{2}{E_2} + \frac{1}{E_1 + \Delta} + \frac{1}{E_2 + \Delta} \right] I \quad (10)$$

with $I = \int (\phi_1^{E1})^* k_z \phi_1^{E2} dz$. This has essentially the same form as the one-band result, but with a mass very different from the band edge value. For M_{12}^x however, the signs are different such that we have an interference

$$\frac{E_p}{6} \left[\frac{-1}{E_1} + \frac{1}{E_2} + \frac{1}{E_1 + \Delta} - \frac{1}{E_2 + \Delta} \right] I \quad (11)$$

The ratio M_{12}^x/M_{12}^z is then small. In the limit that the confinement energies are small compared to the band gap, and writing $E_2 - E_1 = E_{12}$, we find

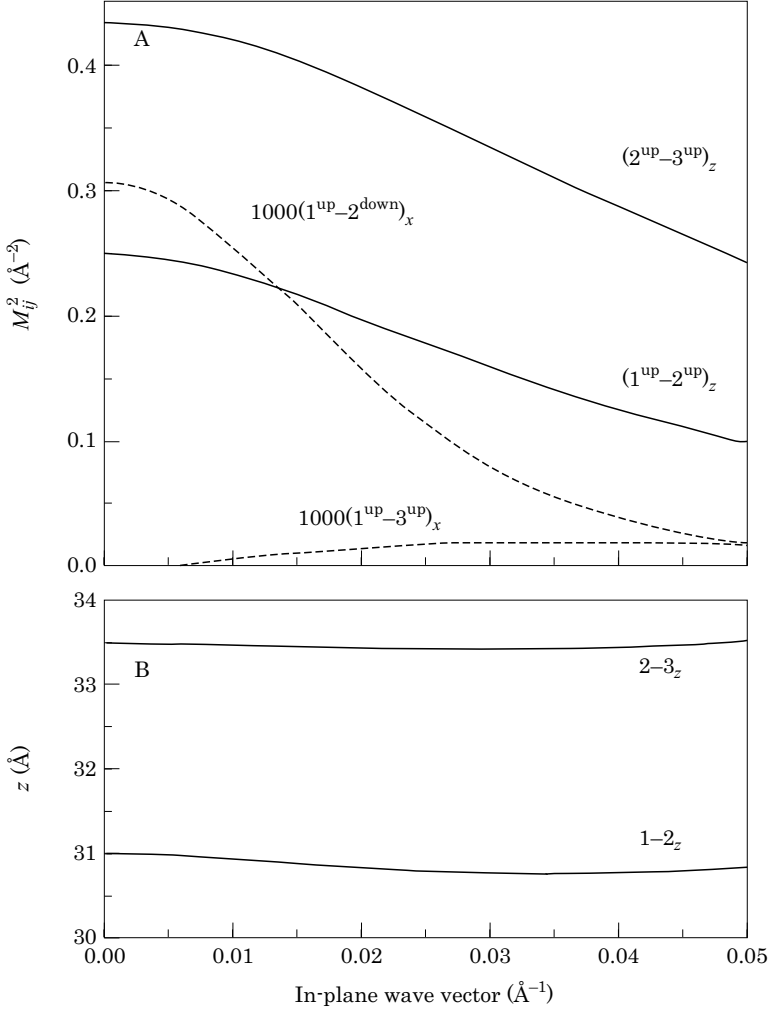


Fig. 4. A, $|M_{ij}^{x(z)}|^2 = |\langle \psi_i | k_{x(z)} | \psi_j \rangle|^2$ (z solid lines and x dotted lines), and B, $\langle z_{ij} \rangle = |\langle \psi_i | z | \psi_j \rangle|$ as a function of the in-plane wave vector k_x for a 150 Å InAs/AlSb quantum well.

$$\left| \frac{M_{12}^x}{M_{12}^z} \right| \simeq \frac{E_{12}\Delta(2E_g + \Delta)}{2E_g(E_g + \Delta)(3E_g + 2\Delta)} \quad (12)$$

which gives approximately $|M_{12}^x : M_{12}^z|^2 = 1 - 2_x : 1 - 2_z \simeq 0.1\%$ for an InAs/AlSb quantum well with $E_{12} \simeq 100$ meV. Note that when $\Delta = 0$ the quantum interference is complete such that $M_{12}^x = 0$.

Exact numerical results for a 150 Å InAs/AlSb quantum well are shown in Fig. 4. Both M_{12}^x and M_{12}^z decrease with increasing k_x as optically-inactive states are mixed in. Fig. 4 shows also M_{13}^x and it is seen to be small, and actually zero at $k_x = 0$; M_{13}^z is negligibly small. We are thus in agreement with Yang *et al.* [3] that $M_{13}^x \gg M_{13}^z$ but this is a somewhat specious comparison as $M_{13}^x \ll M_{12}^z$.

Figure 4 also shows the spatial matrix element $\langle z_{12} \rangle = |\langle \psi_1 | z | \psi_2 \rangle|$ which can be quite generally derived from

$$\langle z_{12} \rangle = \frac{\hbar^2}{m_o} \frac{|M_{12}^z|}{E_{12}} \quad (13)$$

We find that $\langle z_{12} \rangle$ is essentially independent of k_x despite the radical change in the wave function admixture which occurs as k_x is increased. Furthermore, the absolute value (31.0 Å) is very close to that which is obtained from the naive one-band model (33.2 Å). These values are in agreement with the measured values, but again we note that the agreement is better if we assume that the wave function goes to zero at the interfaces ($\langle z_{12} \rangle = 28.8$ Å).

We have not detected any intersubband absorption in parallel excitation experimentally, in accordance with the reasoning above. Experimentally, the conclusion is that $1-2_x:1-2_z < 1\%$. Also, we have not detected $1-3$ in either polarization as expected. Verification that the excitation observed in Fig. 1 comes from z polarization was made by measuring the absorption strength against angle; the results, shown in the inset, can be seen to follow the characteristic $\cos^2\theta/\sin\theta$ dependence [21] (θ is the angle to the normal of the light in the sample). Although these results on parallel excitation are perhaps not at all surprising, other systems based on InGaAs [6–8] and GaAs [9] have apparently given reasonably strong optical activity in parallel excitation. These results are particularly surprising as judged from our own theory in that the $1-2_x:1-2_z$ ratio decreases rapidly with increasing band gap. One possible explanation for the results is that scattering, either from surface roughness or even from the edges of a mesa, scrambles the polarization such that there is a significant polarization along z .

5. Conclusions

The intersubband resonance in highly doped InAs/AlSb quantum wells has been shown to be strongly influenced by collective effects simply from the linewidth. From calculations in the RPA the linewidth reflects the broadening of the levels and not the broadening implied by nonparabolicity in the band dispersion.

The role of nonparabolicity on other aspects of intersubband resonance has also been investigated. The energy is reduced but the matrix element $\langle z_{12} \rangle$ is largely unaffected by nonparabolicity. Although the $1-2$ transition with parallel excitation is not rigorously forbidden, we find that the oscillator strength is small ($< 1\%$) compared to perpendicular excitation. The general conclusion then is that the selection rules and matrix elements from a naive one-band approach are actually remarkably accurate.

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