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Plasmon shake-up effects in quantum-well exciton spectra

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Abstract. We use a model, adopted from the theory of core-hole spectra, to explain the experimentally observed double-peak structures in quantum-well exciton spectra. We also rule out the hypotheses of the peak-splitting being due to any of the following effects: strong electric fields in the sample, doping charge accumulation in the well walls and structures in the well due to the doping-induced deformation of the well potential.

1. Introduction

The system [1–5] we consider here is a GaAs/AlGaAs centre-doped quantum well. The actual samples, used in the experiments to which we refer, have 50 ideally identical, equally spaced, quantum wells (QW). The separation between the wells is big enough for the wells to be considered independent. The doping was performed in a narrow region at the centre of each well and it is in the form of acceptors which means that the majority carriers in the wells are holes.

There are three types of carrier: electrons (e), heavy holes (hh) and light holes (lh). The carrier states are all quantized in the direction perpendicular to the QW plane, but propagate freely in the plane. The states closest to the band extrema dominate the properties. These states are schematically represented in figure 1. At low temperatures only heavy-hole states are occupied. Optical spectra of such a QW are dominated by exciton peaks. There are several types of exciton: hh excitons, lh excitons and excitons bound to acceptors or other defects; there may also be more complex formations like bi-excitons. In photoluminescence (PL) and photoluminescence-excitation (PLE) experiments the peaks from the different types of exciton can be identified.

Within a certain, rather narrow, range of doping levels these peaks are split into pairs [6]. It is with this splitting that we are concerned in this work. The splitting, of roughly 4 meV, is too large to be explained by bi-exciton formation, which would produce a splitting of around 1 meV [6]. We believe that the splitting is due to a shake-up effect caused by the sudden creation of the exciton potential in the heavy-hole gas. This is analogous to the interpretation of the observed effects in absorption and emission experiments on deep core levels in metals; there, the sudden appearance or disappearance of the core-hole potential shakes up the conduction electrons and results in plasmon replication. In section 2 we study the possibility that shake-up effects cause the splitting and obtain a double-peak structure with a splitting of the right order of magnitude.

In section 3 we deal with some other possible explanations of the double-peak structures and demonstrate that the effects are too weak to reproduce the experimental findings. Finally, section 4 contains a summary and conclusions.

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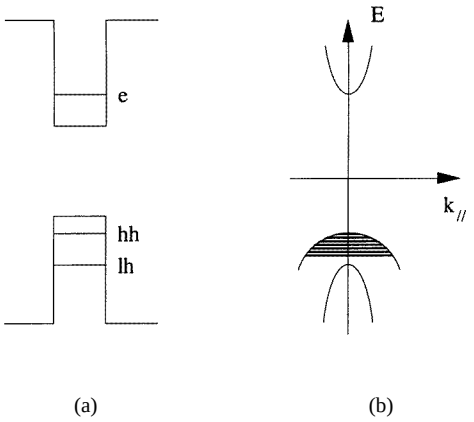

Figure 1. A schematic diagram of the quantum well and the particle states involved. In (a) are indicated the band extrema obtained as a result of the 'particle in a box quantization'. The band structure in the quantum well plane is shown in (b). The shaded area denotes the occupied part of the heavy-hole band.

2. Shake-up effects

The effects we present here are the results of plasmon shake-up. When the exciton is formed in the PLE experiment there is suddenly created a potential in the gas of heavy holes. This potential shakes up the hole-gas and this results in the emission of plasmons. We use a model to describe this that is basically the same as the one used by Langreth [7] for the core-hole problem in the seventies. In connection with this it may also be of interest to the reader to study the problem of the orthogonality catastrophe proved by Anderson [8] and the Mahan–Nozières–de Dominicis theory for the absorption edge singularity [9, 10].

We use the crude assumption that the exciton in the shake-up process does not recoil; its centre of mass remains unchanged and the exciton remains in its ground state. This was also assumed for the core hole. The validity of this assumption here can be questioned, since the exciton is not very heavy compared to the gas of free carriers. Nevertheless we make this assumption and it is needed to make the calculations feasible. In the PL experiments the sudden disappearance of the exciton potential has a similar effect on the hole-gas, namely that plasmons are emitted. Under the assumption that the plasmons all have the same energy the model is easy to solve and it produces a series of peaks, equally spaced, with amplitude given by the Poisson distribution. Depending on the strength of the coupling to the plasmons there may be any number of peaks. In a three-dimensional system the plasmon dispersion curve starts out for small momenta at a finite energy and shows a moderate dispersion. Thus the approximation of a constant plasmon energy is not very severe. In our system, which is quasi-two-dimensional, the plasmon dispersion starts out at zero energy and has a square-root-dependence on momentum. Thus, the assumption of a constant plasmon energy is not useful, if not for some reason one particular plasmon mode were to dominate. This means that we have to go beyond the simplest version of the model.

We use the following model Hamiltonian for the system:

$$H = \varepsilon C_e^\dagger C_e + C_e^\dagger C_e V + H_h$$

where ε, $C_e^\dagger$, C_e, V and H_h are the exciton energy, the creation operator for the exciton, the

destruction operator for the exciton, the interaction potential for the interaction between the exciton and holes and the Hamiltonian for the holes, respectively. The operators V and H_h contain creation and destruction operators for the holes and no exciton operators. We have

$$n_e = C_e^\dagger C_e \qquad [n_e, H] = 0$$

where n_e is the exciton number operator.

In the ground state of the system there is no exciton and the holes are in their ground state. Let us introduce the Hamiltonians

$$H^{(0)} = H_h$$
$$H^{(1)} = \varepsilon + V + H_h.$$

Let $|0\rangle$ denote the ground state of H. It is also the ground state of $H^{(0)}$. Then we have

$$H_h|0\rangle = E_0^h|0\rangle$$
$$H|0\rangle = E_0^h|0\rangle$$
$$H^{(0)}|0\rangle = E_0^h|0\rangle$$

where E_0^h is the ground state energy of the holes. In our choice of ground state the function

$$G^>(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} G^>(t)$$

where

$$G^>(t) = \langle 0|C_e(t)C_e^\dagger(0)|0\rangle$$

is the density of states for the exciton. This is the quantity we need to calculate. Using the fact that there is no exciton in the ground state gives

$$G^>(t) = \langle 0|\mathrm{e}^{\mathrm{i}Ht/\hbar} C \mathrm{e}^{-\mathrm{i}Ht/\hbar} C^\dagger|0\rangle = \mathrm{e}^{\mathrm{i}(E_0^h-\varepsilon)t/\hbar}\langle 0|\mathrm{e}^{-\mathrm{i}(V+H_h)t/\hbar}|0\rangle.$$

It is now time to define our V and the rest of the Hamiltonian. We assume that the structure in the exciton peaks is due to plasmon excitations. The plasmons are collective excitations of the quasi-2D heavy-hole gas. The excitation spectrum of the gas is given by the dynamical structure factor, which is related to the dielectric function according to

$$S(\boldsymbol{q}, \omega) = -\frac{\hbar\kappa}{n v_q} \operatorname{Im} \varepsilon^{-1}(\boldsymbol{q}, \omega)$$

for a semiconductor with background dielectric constant κ. Here $n = N/A$; that is, the average hole density and the dielectric function is that for a quasi-2D hole gas. The structure factor is non-zero in two regions; one region is where hole–electron pairs are excited; the other is the plasmon dispersion curve. We neglect the pair excitations here and only include the plasmons. The plasmons are massless bosons. We get the following effective Hamiltonian:

$$H' = V + H_h = -\frac{1}{A^{1/2}} \sum_{\boldsymbol{q}} g(\boldsymbol{q}) \rho_e^\dagger(\boldsymbol{q})(c_{\boldsymbol{q}} + c_{-\boldsymbol{q}}^\dagger) + \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}}(c_{\boldsymbol{q}}^\dagger c_{\boldsymbol{q}} + \tfrac{1}{2})$$

where $g(\boldsymbol{q})$ is the hole–plasmon coupling constant and the exciton density operator is

$$\rho_e^\dagger(\boldsymbol{q}) = \int \mathrm{d}^3 r\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \sum_j Z_j \delta(\boldsymbol{r} - \boldsymbol{R}_j) = \sum_j Z_j\, \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_j} = \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_h} - \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_e}$$

$$\rho_e(\boldsymbol{q}) = \int \mathrm{d}^3 r\, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} \sum_j Z_j \delta(\boldsymbol{r} - \boldsymbol{R}_j) = \sum_j Z_j\, \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_j} = \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_h} - \mathrm{e}^{-\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{R}_e}.$$

We treat the exciton as a classical particle; that is, the exciton operators are c numbers. Since there is no kinetic energy term for the exciton the Hamiltonian can be diagonalized. This is achieved by using the following unitary transformation:

$$U = \exp\left(\sum_{\boldsymbol{q}} f^{\dagger}(\boldsymbol{q})(c_{\boldsymbol{q}} - c^{\dagger}_{-\boldsymbol{q}})\right)$$

where

$$f^{\dagger}(\boldsymbol{q}) = f(-\boldsymbol{q}) = \frac{g(\boldsymbol{q})}{A^{1/2}\hbar\omega_{\boldsymbol{q}}}\rho^{\dagger}_{e}(\boldsymbol{q}).$$

This leads to

$$UH'U^{\dagger} = \sum_{\boldsymbol{q}} \hbar\omega_{\boldsymbol{q}}(c^{\dagger}_{\boldsymbol{q}}c_{\boldsymbol{q}} + \tfrac{1}{2}) + \Delta\varepsilon$$

where

$$\Delta\varepsilon = -\frac{1}{A}\sum_{\boldsymbol{q}} \frac{|g(\boldsymbol{q})|^2}{\hbar\omega_{\boldsymbol{q}}}\rho^{\dagger}_{e}(\boldsymbol{q})\rho_{e}(\boldsymbol{q}) = -\frac{1}{A}\sum_{\boldsymbol{q}} \frac{2|g(\boldsymbol{q})|^2}{\hbar\omega_{\boldsymbol{q}}}\{1 - \cos[\boldsymbol{q}\cdot(\boldsymbol{R}_e - \boldsymbol{R}_h)]\}.$$

Thus, we see that the ground state of the system with the exciton present is the ground state of the plasmons (the same type of plasmons with the same dispersion as before) and there has been a shift, $\Delta\varepsilon$, in the energy. This shift is the relaxation energy; the gain in energy when the holes relax around the exciton. Also this ground state has no plasmons excited. Let us now return to our Green function

$$G^{>}(t) = \mathrm{e}^{\mathrm{i}(E^{h}_{0} - \varepsilon)t/\hbar}\langle 0|\mathrm{e}^{-\mathrm{i}[H']t/\hbar}|0\rangle.$$

Straightforward, but tedious, manipulations lead to

$$G^{>}(t) = \mathrm{e}^{-\mathrm{i}(\varepsilon/\hbar + \Delta\varepsilon/\hbar)t}\exp\left(-\sum_{\boldsymbol{q}}|f(\boldsymbol{q})|^2(1 - \mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{q}}t})\right).$$

We want the Fourier-transformed version. It is

$$G^{>}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G^{>}(t) = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}(\omega - \varepsilon/\hbar - \Delta\varepsilon/\hbar)t}\mathrm{e}^{B(t)}$$

where the so-called satellite generator is defined as

$$B(t) = -\sum_{\boldsymbol{q}}|f(\boldsymbol{q})|^2(1 - \mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{q}}t}).$$

In the unperturbed case, namely when there is no interaction between the exciton and the plasmons, we have

$$G^{>}_{0}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}(\omega - \varepsilon/\hbar)t} = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G^{>}_{0}(t).$$

We can write

$$G^{>}(\omega) = \int_{-\infty}^{\infty}\mathrm{d}t\,\mathrm{e}^{\mathrm{i}\omega t}G^{>}_{0}(t)\,\mathrm{e}^{C(t)}$$

where

$$C(t) = B(t) - \mathrm{i}\Delta\varepsilon t/\hbar = -\sum_{\boldsymbol{q}}|f(\boldsymbol{q})|^2(1 - \mathrm{i}\omega_{\boldsymbol{q}}t - \mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{q}}t})$$

$$= -\frac{1}{A}\sum_{\boldsymbol{q}}\frac{|g(\boldsymbol{q})|^2|\rho_{e}(\boldsymbol{q})|^2}{(\hbar\omega_{\boldsymbol{q}})^2}(1 - \mathrm{i}\omega_{\boldsymbol{q}}t - \mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{q}}t})$$

In a strictly 2D system the hole–plasmon coupling constant, $g(\boldsymbol{q})$, is found from the identification

$$|g(\boldsymbol{q})|^2\delta(\omega-\omega_{\boldsymbol{q}}) = \frac{v_{\boldsymbol{q}}^{2D}}{\kappa}\delta[\mathrm{Re}\varepsilon^{2D}(\boldsymbol{q},\omega)] = \frac{v_{\boldsymbol{q}}^{2D}}{\kappa}\frac{\delta(\omega-\omega_{\boldsymbol{q}})}{|(\mathrm{d}/\mathrm{d}\omega)(\alpha_0^{2D}(\boldsymbol{q},\omega)/\kappa)|_{\omega=\omega_{\boldsymbol{q}}}}.$$

Thus, the coupling constant is identified as

$$|g(\boldsymbol{q})|^2 = \frac{v_{\boldsymbol{q}}^{2D}}{|(\mathrm{d}/\mathrm{d}\omega)\alpha_0^{2D}(\boldsymbol{q},\omega)|_{\omega=\omega_{\boldsymbol{q}}}}$$

where $\alpha_0^{2D}(\boldsymbol{q},\omega)$ is the polarizability of the hole gas. We use the pure RPA (random phase approximation) expression for this quantity and the plasmon dispersion curve is traced out numerically.

We see that the background dielectric screening has no direct effect. Indirectly, however, it has an effect since the plasmon dispersion curve depends on the screening. Now in a quasi-2D system $v_{\boldsymbol{q}}$ acquires a q-dependent correction factor due to the finite extension of the wavefunctions perpendicular to the 2D plane. This factor appears both in the numerator and in the denominator of the expression for the coupling constant. Thus the factors cancel, but of course the correction factor affects the plasmon dispersion. Thus, it comes into play in the same way as does the background screening.

The wavefunction perpendicular to the well can, for all the three types of carrier entering the present problem, to a good approximation be represented by a cosine function whose wavelength is equal to twice the well width. Thus the two-dimensional Fourier transform of the Coulomb potential is replaced according to

$$v_{\boldsymbol{q}}^{2D} = \frac{2\pi e^2}{q} \Rightarrow v_{\boldsymbol{q}}^{2D}\left(\frac{2}{\pi}\right)^2\int_{-\pi/2}^{\pi/2}\mathrm{d}\varphi\int_{-\pi/2}^{\pi/2}\mathrm{d}\varphi'\cos^2(\varphi)\,\mathrm{e}^{-q|\varphi-\varphi'|\mathrm{width}/\pi}\cos^2\varphi'.$$

The quasi-2D character of the system also means that heavy holes can be excited into the light-hole band and into more bands further down in the valence-band well. Thus there are inter-band transitions. If these are included they have the effect that the plasmon dispersion is deformed and pushed somewhat downwards and kept below the region of inter-band transitions. We have not taken this effect into account here. We have neglected inter-band transitions altogether.

Now, we need to determine $|\rho_e(\boldsymbol{q})|^2$. For the ground state of an exciton we have

$$\Phi(r) = \frac{2^{3/2}}{\sqrt{\pi}a}\,\mathrm{e}^{-2r/a} \qquad n(r) = \frac{2^3}{\pi a^2}\,\mathrm{e}^{-4r/a} \qquad a = \frac{\hbar^2\kappa}{m_{red}e^2}$$

where $\Phi(r)$, $n(r)$ and a are the wavefunction, the probability density and effective Bohr radius, respectively. The distance r is here the distance between the electron and hole. The contribution to the exciton spectra from plasmons with wavevector $\boldsymbol{q}$, if the electron and hole had specific positions in space with the separation given by $\boldsymbol{r}$, was above found to be determined by

$$|\rho_e(\boldsymbol{q})|^2 = 2[1-\cos(\boldsymbol{q}\cdot\boldsymbol{r})].$$

The exciton wavefunction is built up by many possible configurations of the electron and hole positions. The probability distribution for a separation r is given by $n(r)$. The probability distribution is spherically symmetrical. The net contribution for the exciton is given by

$$|\rho_e(\boldsymbol{q})|^2 = \int_0^\infty \mathrm{d}r\int_0^{2\pi}\mathrm{d}\varphi\frac{2^3}{\pi a^2}r\,\mathrm{e}^{-4r/a}2[1-\cos(qr\cos\varphi)].$$

Now, we have everything we need to calculate the exciton excitation spectra. If we use the unperturbed exciton energy as our zero of reference we get

$$D(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{\mathrm{i}\omega t} \mathrm{e}^{C(t)} = \int_{-\infty}^{\infty} \mathrm{d}t \exp\left(\mathrm{i}\omega t - \frac{1}{A} \sum_{\boldsymbol{q}} \frac{|g(\boldsymbol{q})|^2 |\rho_e(\boldsymbol{q})|^2}{(\hbar\omega_{\boldsymbol{q}})^2} (1 - \mathrm{i}\omega_{\boldsymbol{q}} t - \mathrm{e}^{-\mathrm{i}\omega_{\boldsymbol{q}} t}) \right).$$

Let

$$a(t) = \frac{1}{A} \sum_{\boldsymbol{q}} \frac{|g(\boldsymbol{q})|^2 |\rho_e(\boldsymbol{q})|^2}{(\hbar\omega_{\boldsymbol{q}})^2} [1 - \cos(\omega_{\boldsymbol{q}} t)]$$

$$\Delta\varepsilon = -\frac{1}{A} \sum_{\boldsymbol{q}} \frac{|g(\boldsymbol{q})|^2 |\rho_e(\boldsymbol{q})|^2}{(\hbar\omega_{\boldsymbol{q}})}$$

$$b(t) = \frac{1}{A} \sum_{\boldsymbol{q}} \frac{|g(\boldsymbol{q})|^2 |\rho_e(\boldsymbol{q})|^2}{(\hbar\omega_{\boldsymbol{q}})^2} \sin(\omega_{\boldsymbol{q}} t).$$

Then we have

$$D(\omega) = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{[\mathrm{i}\omega t - a(t) - \mathrm{i}\Delta\varepsilon t/\hbar - \mathrm{i}b(t)]} = \int_{-\infty}^{\infty} \mathrm{d}t\, \mathrm{e}^{-a(t)}\, \mathrm{e}^{\mathrm{i}[\omega t - \Delta\varepsilon t/\hbar - b(t)]}$$
$$= 2 \int_{0}^{\infty} \mathrm{d}t\, \mathrm{e}^{-a(t)} \cos[\omega t - \Delta\varepsilon t/\hbar - b(t)].$$

The experimental peaks have a finite width, W_p, which is due to combined effects from experimental broadening, broadening due to pair excitations and broadening due to the finite life-time of the exciton. We simulate this (this is not entirely strict) by introducing an exponentially decaying factor into the integrand. This procedure also improves the numerical accuracy and reduces the computer time. The final result is

$$D(\omega) = 2 \int_{0}^{\infty} \mathrm{d}t\, \mathrm{e}^{-W_p t/2\hbar} \mathrm{e}^{-a(t)} \cos[\omega t - \Delta\varepsilon t/\hbar - b(t)].$$

In figure 2 we give our numerical results for a light-hole exciton, at different doping densities in the range within which the double-peak structure is found experimentally. We have assumed that W_p is 1.7 meV, which is the value found from the experiments.

The area under each curve is 2π. There are never more than two peaks, in agreement with experiments. It can be seen that the splitting increases with doping level. For the highest doping levels the splitting is larger than that in the experiments. Inclusion of inter-band transitions in the dielectric function for the quasi-2D hole gas would probably prevent this discrepancy. It is not possible to find out from the experiments which of the two peaks is the largest; this varies depending on which recombination channel is chosen as the detection channel.

We mentioned in section 1 that the separation of the wells is big enough for the wells to be considered independent. However, plasmons of long wavelength are sensitive to coupling between wells since the fields from these plasmons extend long distances in the direction perpendicular to the well planes. Thus, one has to be careful in neglecting the coupling when plasmons are involved. We made a rough estimate of the effect of the coupling between neighbouring wells in the following way. We studied two wells separated by 300 Å, which is the actual separation between the wells in the samples. The coupling between two wells is determined by the factor $\exp(-2qd)$, for the wavenumber q and separation d. In our calculation the whole plasmon branch contributes to the spectrum, but we here make the assumption that the plasmon with energy equal to the separation between the two peaks dominates. For our three samples with doping densities 1×10^{11},

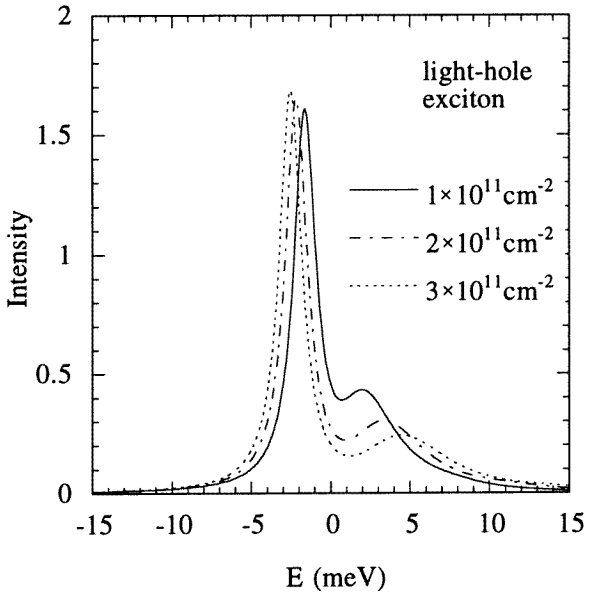

Figure 2. The predicted light-hole PL peak for samples with doping concentrations 1×10^{11} cm^{-2} (full curve), 2×10^{11} cm^{-2} (chain curve) and 3×10^{11} cm^{-2} (dotted curve). In each curve the rightmost weaker peak is due to plasmon shake-up processes. It contains contributions from processes whereby any number of any of the different plasmons have been excited. All curves are relative to the position without the plasmon interactions. The main peak is shifted downwards in energy by the interactions but the centre-of-mass of the spectrum remains unchanged.

2×10^{11} and 3×10^{11} cm^{-2}, we found the exponential factors to be 0.006, 0.002 and 0.001, respectively, for the dominating plasmon. Thus, this demonstrates that the coupling is very weak. For two wells at large separation there are two degenerate plasmon branches. These are split when the separation between the wells is reduced and the size of this splitting is an alternative measure of the effect of the coupling. We found that this splitting is 0.1 meV for all three samples, which can be considered negligible. In the case of 50 wells the effect of the coupling will probably be that the plasmon branch is replaced by a band of plasmons with an energy width of roughly 0.1 meV. Since all plasmons contribute and the spread in plasmon energy is larger for plasmons with longer wavelengths the detailed shape of the second peak in the spectra could be slightly modified by the coupling between the wells. We leave this for a possible future extension of the theory.

3. Effects of a strong electric field, doping charge accumulation and well-potential deformation due to the centre doping

An electric field perpendicular to a quantum well tilts the bottom of the well. This has two effects: the energy separation between the states in the conduction-band and valence-band wells is changed, resulting in an energy shift of the PL peaks; and the electron and hole wavefunctions are spatially shifted in different directions along the field direction, leading to a reduction in the overlap and hence a suppression of the luminescence intensity. This is known as the confined Stark effect [12–14].

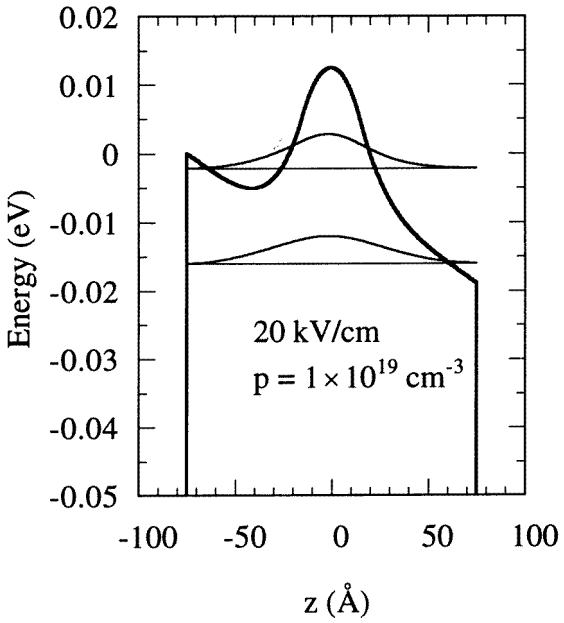

Figure 3. The actual valence-band quantum well for a heavily doped sample with a doping concentration of 1×10^{19} cm^{-3} and an external electric field of 20 kV cm^{-1}. Since the doping is homogeneously distributed within a layer of 30 Å at the centre of the well the 2D doping concentration is 3×10^{11} cm^{-2}. The horizontal lines are the band extrema for the two types of hole band and the corresponding perpendicular wavefunctions squared are shown, representing the corresponding carrier distributions perpendicular to the well plane.

The actual system we consider consists of 50 quantum wells in parallel. All of the wells are intended to be identical. If all of the wells experience the same field strength then the experimental exciton peaks, which have contributions from all of the wells, are shifted in energy. If the field strength varies from well to well one would imagine that the result would be a broadening of the exciton peaks and not a splitting of each peak into two, as is found experimentally. The splitting suggests that there are two field strengths rather than a distribution of field strengths in the sample. One could imagine that the outermost wells might experience a different field strength than do the majority of the wells in the centre. If this were the case the intensity of one of the peaks would be just some few per cent of that of the other. This is not observed, though. Also the fact that the splitting occurs just for samples within a narrow range of doping densities militates against the explanation of the splitting as being due to two different field strengths in the sample. We are instead looking for a splitting of the peaks, within each single well—a splitting that depends on the doping concentration, perhaps in combination with an external field.

Each QW is 150 Å wide and a layer of roughly 30 Å in the centre of each well is p-type doped. This doping is the source that provides the holes for the hh band. When the acceptors are ionized the holes are distributed within the well but the ions are still confined to the narrow region in the centre of the well. Thus there is a re-distribution of charge or a charge separation in the well. For heavy doping the well potential is not as simple as that sketched in figure 1. The charge separation leads to a deformation of the bottom of

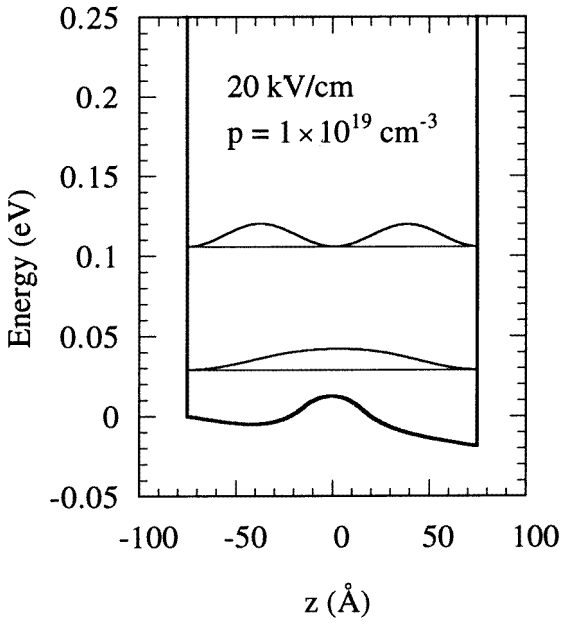

Figure 4. The actual conduction-band quantum well for the same sample as in figure 3. The horizontal lines are the band extrema for the two lowest electron bands and the corresponding perpendicular wavefunctions squared are shown, representing the corresponding carrier distributions perpendicular to the well plane.

the well (or of the top, depending on how we look upon the valence-band well). A 'valley' is formed. In the conduction band a corresponding barrier is formed. These structures, if they are important enough, could lead to a dramatic change in the quantized levels. In the conduction band one may imagine that there are two levels below the top of the barrier, one on each side. What would actually happen in that situation if the well were symmetric is that there would be one symmetrical and one anti-symmetrical solution. The solutions would have slightly different energies. If a strong electric field were to act perpendicular to the well plane the splitting between the levels would increase. This would mean that there are two excitons with different energies since there would be two different electron states that can participate in the exciton formation. It is impossible to know whether this is a plausible explanation before the actual calculations have been done.

There is also another possible explanation, namely the following. When the sample is grown there is always a tendency for the doping atoms to be dragged along with the surface growth boundary. As a result a fraction of the doping atoms is accumulated at one of the QW walls. We have also modelled this and found that the effect is very similar to that of an applied electric field.

In both these cases we start with a guessed potential, then solve the Schrödinger equation numerically to find the energy levels and wavefunctions. Then we determine the occupation numbers for the bands in accordance with the actual temperature. This gives the charge density. Then, with the help of the Poisson equation we calculate the potential. We repeat this procedure in iteration until everything converges. In order to find convergence we have to use a sensitive way to include a mixture of the old and new potentials at each step of

the iteration, otherwise results from the different iterations will oscillate. The results for an applied electric field of 20 kV cm^{-1} are shown in figures 3 and 4 for a sample with a doping density of 1×10^{19} cm^{-3}, which corresponds to a 2D density of 3×10^{11} cm^{-2}. Figures 3 and 4 are for the valence and conduction bands, respectively.

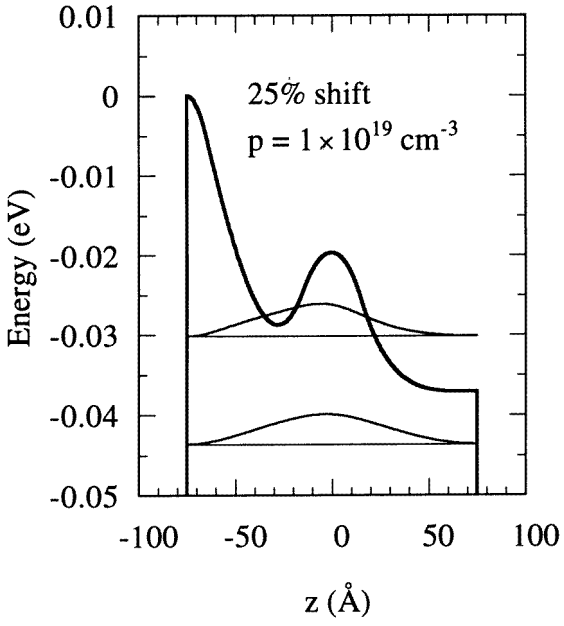

Figure 5. The same as figure 3 except that here there is no external field present. Instead 25% of the acceptors have been removed from the doped region in the centre and put at the position of the left-hand well wall.

We note that the re-distribution of the carriers leads to a weakening of the effective field by roughly one third. We also note that the barrier in the conduction band well is too weak to make the two levels nearly degenerate. All levels are above the barrier. However, we also find that the valence band will have a double-valley structure at this high a field strength, but the structure is too weak to lead to a degeneracy. We have also performed calculations at 50 kV cm^{-1} and there is still no degeneracy or near degeneracy.

In figure 5 we present the result for the valence-band QW when we have no applied field, but instead have let 25% of the doping atoms be accumulated at the left-hand wall of the well. The result looks much the same as it does for an applied field of 50 kV cm^{-1}. We see that there is no tendency towards a degeneracy. The highest hole band has moved up from the valleys. Thus, we have found that neither a strong electric field nor a re-distribution of the doping atoms can explain the peak splitting found in the experiments.

4. Summary and conclusions

We have tested several different explanations for the splitting of the peaks in exciton spectra from p-type centre-doped GaAs/AlGaAs quantum wells. The barrier and valley formed in the conduction- and valence-band wells due to the doping were found to be too weak to cause the splitting. An applied electric field perpendicular to the well planes caused a

double-valley structure in the valence-band well. If two hole states were trapped in this double-valley structure, one in each valley, this could possibly cause the splitting. We found that the structure is too weak to trap two hole states. Accumulation of dopants at one of the well walls had an effect similar to that of an applied field and was found not to be capable of causing the splitting.

We also tested a dynamic explanation for the splitting, namely that the splitting is caused by shake-up effects in the excitation and de-excitation processes. When the exciton is formed the sudden appearance of the exciton potential causes a shock on the hole gas. This results in emission of plasmons; in the present system these are quasi-2D plasmons. We used a model developed for the core-hole problem to treat these effects. We found a double-peak structure with a splitting of the right order of magnitude. We found just two peaks, as in the experiments, although the model could have produced any number of peaks. At the high-doping limit the splitting is larger than the experimental values. An explanation for this discrepancy might be that we have not taken into account the effects of inter-band transitions. Inclusion of these should force the plasmon dispersion curve to stay below the inter-band electron-hole–pair continuum and thereby counteract an increase in the splitting for higher doping concentrations. We think that the plasmon shake-up effect is a plausible explanation for the experimentally observed effects.

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