Lightly doped and compensated quantum wells: The density of states in the dipole model

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We present a calculation of the density of states (DOS) of electrons bound to donor impurities in a lightly doped and compensated quantum well. We use a quasiclassical treatment suitable for low compensation in which we apply the dipole model. If the full electron-electron Coulomb interactions were taken into account, instead of the short-range dipole interaction, a Coulomb gap should appear around the Fermi level. But this model is able to describe the small peak of unoccupied states that appear, as a result of compensation, in the high-energy side of the DOS. In this work we show how the additional peak varies with the well width, impurity concentration, and compensation in the small-impurity-concentration limit.

It is well established by now that a gap in the density of states (DOS) occurs at the Fermi level in a lightly doped and compensated semiconductor. In the past Efros, Van Lien, and Shklovskii[1] have calculated the DOS, using a numerical simulation method due to Baranovskii *et al.*[2] to obtain the ground state of this system, in the so-called classical impurity band model. In fact, when the impurity concentration is very small the electrons are in the completely localized regime. The overlap of the wave functions representing the one-electron ground state is negligible as the average distance between impurities is much greater than the localization length. In that case the donors and acceptors can be assumed as point charges.[3]

At sufficiently low temperatures all acceptors are ionized. If n_i represents the occupancy of a donor i, $r_{i\mu}$ stands for the distance between that donor and an acceptor μ; the system can be described by the classical Hamiltonian:

$$\mathcal{H}=\tfrac{1}{2}\sum_{\substack{i,j\\(i\neq j)}}\frac{e^2}{kr_{ij}}(1-n_i)(1-n_j) -\sum_{i,\nu}\frac{e^2}{kr_{i\nu}}(1-n_i)+\tfrac{1}{2}\sum_{\mu,\nu}\frac{e^2}{kr_{\mu\nu}} . \quad (1)$$

For low compensation the ionized donors are those near an acceptor, resulting in unoccupied electron states with higher energies than those occupied at neutral donors.

It turns out that a simple way to treat that problem analytically is the dipole model: each acceptor ionizes its nearest-neighbor donor and the pair does not perturb the states of neutral donors as its potential rapidly decays. A bandwidth appears in this additional peak at the DOS located at e^2/kr, where r is the distance between atoms in the pair, corresponding to the unoccupied "dipole states." The spread in energy is due to randomness in the dipole moment. Using this simplified picture, a two-peaked DOS comes out: a deltalike peak due to states in neutral donors and a separated broad peak of the unoccupied states in the donors forming dipoles with ionized acceptors. Actually, fluctuations of the electrostatic potential at the neutral donors are responsible for a considerable broadening of the delta peak. However the DOS does not change qualitatively and indeed the dipole model was shown[4] to give very good results in the calculation of the electric field distribution.

In this work we extend the dipole model to treat a lightly doped and compensated semiconductor heterostructure: the $Ga_{1-x}Al_xAs/GaAs$ quantum well (QW). We assume that hydrogenlike donor and acceptor impurities occur in the small gap layer of GaAs. The impurity concentration is allowed to vary along the QW according to a normalized profile $P(Z_i)$, where Z_i is the distance to the center of the well. We assume, per unit volume, N_D donor impurities, and $N_A=KN_D$ acceptors—K is the compensation—in the QW of width L and define the effective two-dimensional concentration $n_D=N_DL$.

The single-impurity problem has been treated variationally by Bastard.[5] His calculations, although they have been subsequently extended to include several improvements, present the right qualitative behavior and are accurate within 10%. In a way, we can express the ground-state energy of an electron bound to a shallow isolated donor as

$$E(Z_i;L)=a(L)Z_i^4+b(L)Z_i^2+c(L) , \quad (2)$$

where we have fitted Bastard's results with a fourth-order polynomial. If we measure (as we do hereafter) the energies in effective rydbergs and distances in the effective Bohr radius ($1\text{Ry}^*\cong 5.8$ meV and $a_0^*\cong 100$ Å for GaAs, respectively) we obtain the parameters shown in Table I, where we have made $E(0;L)=0$. So for low concentration and uncompensated samples, the DOS becomes

TABLE I. Coefficients of the fourth-order polynomial adjusted to fit Bastard's eigenvalues of the isolated-impurity problem in the QW. Units are so that, if Z_i is computed in units of a_0^*, Eq. (2), with the above coefficients, gives the energy in Ry* [$C(L)=0$].

	$L=1$	2	3	4	(a_0^*)
a	−14.26	−0.788	−0.128	−0.030	
b	7.506	1.706	0.676	0.336	

$$D_L(\varepsilon)=\eta_D\int P(Z_i)\delta(\varepsilon-E(Z_i;L))dZ_i\ . \tag{3}$$

In the case of uniform distribution inside the well, $P(Z_i)=L^{-1}$, and using Eq. (2) we obtain

$$D_L(\varepsilon)=\eta_D(|a_L|/2b_L^3)^{1/2}\{[1-f_L(\varepsilon)^{1/2}]f_L(\varepsilon)\}^{1/2}\ , \tag{4}$$

with

$$f_L(\varepsilon)=1-4|a_L|\varepsilon/b_L^2\ , \tag{4a}$$

where $a_L=a(L)$ and so on. Observe that Eq. (4) diverges at $\varepsilon=0$ what is due to the minimum at this energy. The structure of this DOS has already been extensively discussed.[5–7]

Let us assume now that the impurities (both donors and acceptors) are distributed only within a thin layer around Z_i of width Δ inside the well and in such a concentration that $\Delta \ll L \ll R_0$, where R_0 is the average separation between impurities. Then each donor-acceptor pair in the QW contributes to the DOS with energy $E(Z_i;L)+2/r$ giving origin to the upper branch of the DOS. So,

$$D(\varepsilon;Z_i)=(1-K)D^{(1)}(\varepsilon-E(Z_i;L))+KD^{(2)}(\varepsilon-E(Z_i,L))\ , \tag{5}$$

with

$$D^{(1)}(w)=\eta_D\delta(w) \tag{5a}$$

and

$$D^{(2)}(w)=\eta_D\int p(r)\delta\left[w-\frac{2}{r}\right]dr\ , \tag{5b}$$

where now $\eta_D=N_D\Delta$ and $p(r)$ is the probability for the donor pairs to be separated by a distance r and is given by the Poisson distribution

$$p(r)=2\pi r\eta_D e^{-\pi r^2\eta_D}\ . \tag{6}$$

The above two-dimensional limit approximation cannot be used if $\Delta \lesssim L$ and the problem then becomes much more complicated. Some of us[7,8] have treated this case in a more severe circumstance, namely, for intermediate concentration, when the overlap between the electrons wave functions cannot be neglected. We have shown[8] in that case that the transfer matrix, or the hopping, between impurity sites i and j is not very sensitive to the positions Z_i and Z_j up to an impurity layer width of the order of $L/2$. Then, we could consider for the DOS the approximated following expression:

$$D(\varepsilon)=\int P(Z_i)D(\varepsilon;Z_i)dZ_i\ , \tag{7}$$

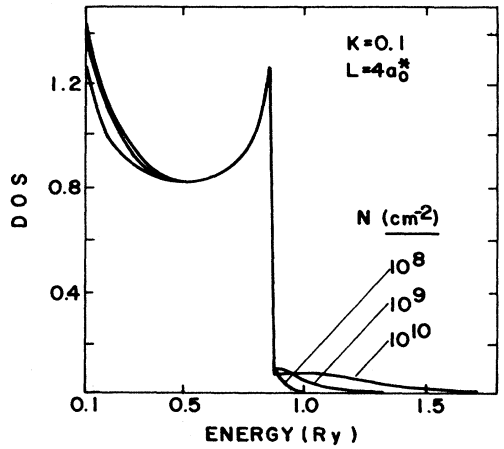

FIG. 1. Density of states (DOS) per donor as calculated by Eq. (8) for the concentrations (a) 10^8 cm^{-2}, (b) 10^9 cm^{-2}, and (c) 10^{10} cm^{-2}. We used $L=4a_0^*$ and compensation $K=0.1$.

where $D(\varepsilon;Z_i)$ is the DOS calculated as if all impurities were located at Z_i. To follow this reasoning in the case of lightly doped QW's one must treat the dipole energy $2/r_{ij}$ as was done for the hopping. Fortunately it turns out that in this case the above approximation [Eq. (7)] is much better. In fact, within our precision (10^{-4} Ry*), $2/r_{ij}$ does not change with $|Z_i-Z_j|$ because we are always considering situations so that $\eta_D^{-1/2}\gg L$.

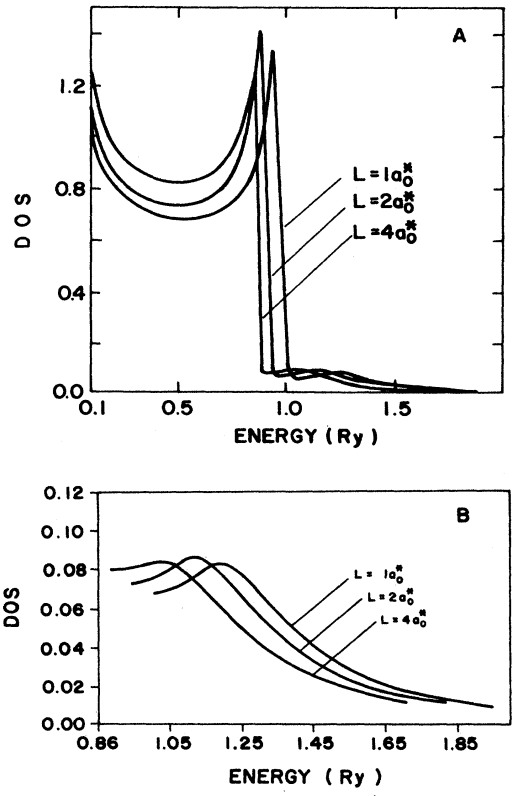

FIG. 2. The DOS now for different well widths L (a). In this case $\eta_D=10^{10}$ cm^{-2} and $K=0.1$. (b) shows detail of the extra peak of empty dipole states.

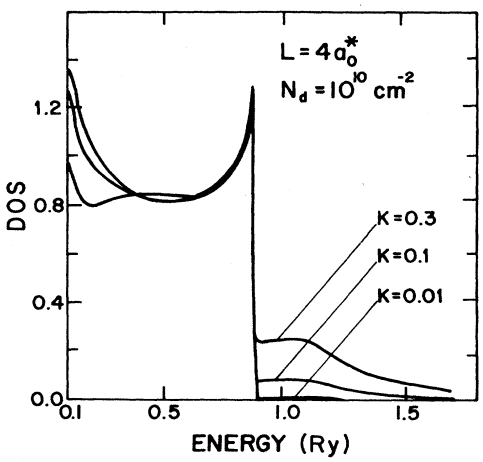

FIG. 3. Results of the DOS [Eq. (8)] for the compensations $K=0.1$, 0.1, and 0.3 with $L=4a_0^*$ and $\eta_D=10^{10}\ \mathrm{cm}^{-2}$.

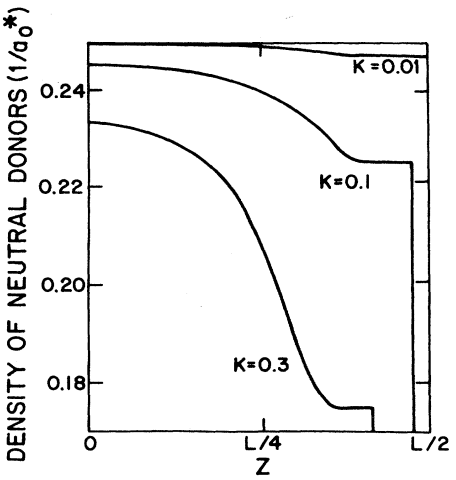

FIG. 4. Distribution of neutral donors inside the quantum well as varying with the compensation. The well width used was $L=4a_0^*$ and $\eta_D=10^{10}\ \mathrm{cm}^{-2}$.

Then, we can approximate the total DOS for the lightly doped and compensated QW with the following two branches:

$$D_L(\varepsilon)=(1-K)D_L^{(1)}(\varepsilon)+KD_L^{(2)}(\varepsilon)$$
$$=\int P(Z_i)D(\varepsilon;Z_i)dZ_i\ , \tag{8}$$

where $D(\varepsilon;Z_i)$ is the one given by Eq. (5), $D_L^{(1)}(\varepsilon)$ by Eq. (3) and

$$D_L^{(2)}(\varepsilon)=\eta_D\int dZ_i\,P(Z_i)\int P(r)\delta(\varepsilon-E(Z_i;L)-2/r)dr\ . \tag{9}$$

For the uniform distribution $P(Z_i)=L^{-1}$, $D_L^{(1)}$ is given by Eq. (4) and

$$D_L^{(2)}(\varepsilon)=\frac{2\pi\eta_D^2}{L}\int_0^{L/2}\exp\left[-\pi\eta_D\left[\frac{2}{\varepsilon-E(Z_i;L)}\right]^2\right]\times\left[\frac{2}{\varepsilon-E(Z_i;L)}\right]^3\times\Theta(\varepsilon-E(Z_i;L))dZ_i\ . \tag{10}$$

Figures 1–3 show the calculated total DOS [Eq. (8)] for several impurity concentrations, well widths, and compensations, respectively. We have assumed in all situations a uniform profile. All the DOS are normalized to 1. We can see that the principal effect of a small compensation on an n-type doped QW as revealed by the above calculations, is the formation of a small broad peak at higher energies.

It is important to observe that the energy in the dipole states which is in the average $2\eta_D^{1/2}$ above that of the neutral impurity is, at the maximum, of the order of 0.1 Ry*. This is quite small as compared with the spread in energy only due to the randomness in Z_i (independent in the compensation) which is itself of the order of 1 Ry*. Due to this fact, most of the second branch of the DOS overlaps with the first one, meaning that some dipole states will be occupied, preferably near the center of the well (as shown in Fig. 4) and then isolated point charges will occur. The peak corresponding to unoccupied dipole states is expected to be well described in our calculations. The peak should be observed in experiments at very low temperatures and its maximum occurs at 1.04 and 0.87 meV separated from the nearest-neighbor peak for $L=1a_0^*$ and $4a_0^*$, respectively, with $n_D=10^{10}\ \mathrm{cm}^{-2}$ and $K=0.1$.

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