Lightly doped and compensated quantum well: A Monte Carlo simulation

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We analyze a lightly doped and compensated quantum well within a semiclassical impurity-band model. We use a Monte Carlo simulation to study the single-particle density of states (DOS) in an n-type $Ga_{1-x}Al_xAs/GaAs$ infinite well. We also investigate the Fermi level, the charge distribution, and the distribution of the electric fields at neutral donors. The interplay of the confining potential and the compensation in these systems is discussed and found to greatly influence the impurity-band structure. The latter is shown to be not appreciably dependent on the well width L, at least in the range from $L=1$ to 4 effective Bohr radii. A Coulomb gap was always observed to occur in the DOS. Its power law is shown to have a two-dimensional signature of the bound-electron system. The charge distribution is shown to be potentially useful for device diagnosis. The whole range of compensations is investigated, and we show results for superficial concentrations of 10^8 and 10^{10} donors per cm^2.

I. INTRODUCTION

The development of powerful techniques for composition-controlled, pure crystal growths is important in material science. In order to achieve further improvements, a better understanding of new materials such as highly pure semiconductor heterostructures is required. At low temperatures, these heterostructures are characterized by their impurity bands. In this paper we present a thorough analysis of a lightly doped and compensated n-type quantum well (QW) of $Ga_{1-x}Al_xAs/GaAs$. We investigate, by computer simulation, the one-electron density of states (DOS) for donors. We also obtain the Fermi level, the charge distribution inside the QW, and the distribution of the electric field at the neutral-donor sites. We assume the impurities to lay inside the QW, i.e., inside the GaAs layer. We also consider—although this condition may be relaxed—uniform impurity distribution. Then, the system is characterized by the QW width L, the degree of compensation $k \leq 1$, and the donor concentration (per unit area) n_d. We show the results for the whole range of compensation and for realizable values of L and n_d. Similar calculations performed in bulk semiconductors[1,2] had great success in understanding the properties of those materials in the limit of light doping. They provided the basic ingredients to study the intra-impurity absorption line broadening to be used as a powerful method for pure semiconductor diagnosis.[3,4]

Doped semiconductors have long been of great interest for their technological applications. They also constitute excellent examples of disordered systems useful for the sake of studying fundamental phenomena, such as metal-nonmetal transitions (MNM). In fact, the theory of disordered systems is not complete yet. Effects of the electron-electron interaction together with disorder must be taken into account by any theory of the MNM transition.[5,6] Important advances along these lines have been done quite recently for the metal side of the transition for bulk and low-dimensionality systems.[7] In the insulator phase, the electrons are assumed to occupy localized states. In lightly doped semiconductors where we are far from the MNM transition, the interimpurity distance is much larger than the decay constant of the electron wave function or the effective Bohr radius, so the electrons are completely localized. In this case the compensation provides a way for varying the disorder. Efros, Shklovskii, and co-workers[2] have been investigating these systems for some time. Using an algorithm introduced by Baranovskii, Efros, Guelmont, and Shklovskii (BEGS) (Ref. 8) they performed a series of computer experiments which, among other things, proved the existence of a Coulomb gap in the single-particle DOS, in accordance with the theory of Efros and Shklovskii (ES).[9] The Coulomb gap appears due to the long-range character of the electron-electron Coulomb interaction between localized states. The way the DOS approaches zero at the Fermi level depends on the dimensionality of the system. The Coulomb gap manifests itself in the low-temperature conductivity of these disordered systems. A more direct observation, however, was done by Davis and Franz[10] in photoemission data of sodium tungsten bronzes. Recently, Biskupski[11] measured the resistivity of InP in a magnetic field and observed a temperature dependence in agreement with the existence of a Coulomb gap. In our calculations of the QW we have observed the Coulomb

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gap for different combinations of L, k, and n_d. We also show in this paper that for L in the range between 1 and $4a^*$ (effective Bohr radius) the Coulomb gap has a two-dimensional signature.

In the present calculation, the main difference between the QW and the bulk semiconductor is that in the former the electron binding energy depends on the impurity position along the growth direction (z axis). The dependence comes out of the breaking of crystal symmetry due to the confining potential of the $Ga_{1-x}Al_xAs$ and GaAs interfaces. The binding energy decreases as the impurity moves from the center to the interfaces. Also, it decreases by increasing the well width. The experiments of Shanabrook and Comas[12] and also Jarosik *et al.*[13] are in qualitative agreement with effective-mass calculations for isolated impurities. For quantitative agreement, however, we need to go beyond and incorporate interimpurity interactions and a proper way to treat disorder. It turns out that, in the lightly doped regime, the main effect which controls both the interaction and the disorder source is the compensation. Its effect on bulk semiconductors is very well understood now and the Monte Carlo simulation introduced by Efros and co-workers has shown to be the only method able to describe satisfactorily the whole spectrum of compensation. We use that same method in the lightly doped QW's. It is worthwhile to mention that Duffield *et al.*,[14] investigating superlattices, reported far-infrared-spectroscopy data which show inhomogeneously broadened absorption lines related to the distribution of neutral donors inside the wells. As the binding energy has a maximum at the well's center, neutral impurities are more likely to occur there in order to minimize the system's energy. We go further and show that the charge distribution is smooth (due to Coulomb interaction) and its width and decay rate depend, respectively, on the compensation and impurity concentration.

The DOS of uncompensated QW's has already attracted much attention.[15–17] In Ref. 17 it was discussed in detail in both low and intermediate concentration regimes. In the first case we use the isolated impurity model and, instead of the δ-function-like DOS which occurs in bulk semiconductors, we find a broadened DOS with a double peak structure, as shown in Fig. 1. The peaks occur in the extremes of the energy range. There it is shown schematically how the single-site energy varies with the impurity z coordinate. As minority impurities cannot be avoided, their effects in the optical-electronic properties of the QW must be considered. We show in this paper that these effects are very important for lightly doped QW's. The uncompensated bandwidth in this regime is due only to diagonal disorder and it is typically, for GaAs QW's, of the order of 1 Ry* ($\simeq 5.8$ MeV). When there is compensation, an extra broadening mechanism is the random Coulomb interaction which involves energies typically of the order of $2\sqrt{n_d}$Ry*, where n_d is given in effective atomic units (a^{*-2}). For $n_d = 10^{10}$ cm^{-2}, for instance, this energy is ~ 0.2 Ry*. However, compensation also allows the electrons to move to the center of the well by the influence of the confining potential. This increases the Coulomb interaction. The interplay of compensation and confinement largely determines the properties of lightly doped QW's.

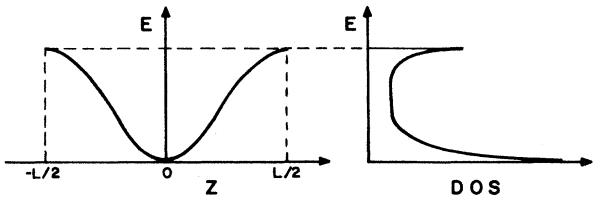

FIG. 1. Schematic drawing of the single-site energy dependence with the z coordinate of the impurity. The QW has width L and interfaces at $z = \pm L/2$. With the same energy axis, the structure of the uncompensated DOS is also shown.

In the next section we describe the model and the numerical approach. In Secs. III–VI we discuss the DOS, the Coulomb gap, the charge distribution, and the electric-field distribution, respectively.

II. THE SEMICLASSICAL IMPURITY-BAND MODEL (SCIB) AND THE MONTE CARLO SIMULATION

The model we use in this work to describe impurities is an extension of the classical impurity-band model (CIB) (Ref. 18) used for QW's in doped semiconductors in the low-concentration limit. We assume the impurity concentration to be low so that electron states in the N donors and kN acceptors are completely localized. At low temperature, double occupancy is very unlikely, so all acceptors—and the same number of donors—are ionized. Since, in this regime, overlaps between intersite impurity states are negligible, we can treat our system as consisting of point charges.[18] In this case the energy of an electron bound to a donor at site i is, in effective atomic units, given by

$$E_i = -\sum_{j(\neq i)}^{N} \frac{2(1-n_i)}{r_{ij}} + \sum_{\nu=1}^{kN} \frac{2}{r_{i\nu}} + E_L(z_i) , \tag{1}$$

where r_{ij} stands for the distance from donors at i and j, and $r_{i\nu}$ for a donor at i and an acceptor at ν. The occupancy n_i is either 0 or 1, for unoccupied or occupied sites, respectively. The quantum-mechanical signature appears in the model through the ground-state energy E_L, which depends on position due to the confining potential, $V_L(z)$:

$$E_L(z_i) = \left\langle \psi \left| -\nabla^2 \frac{-2}{[x^2+y^2+(z-z_i)^2]^{1/2}} + V_L(z) \right| \psi \right\rangle . \tag{2}$$

The energy is reckoned from the bottom of the well. It is important to notice that, in the completely localized and singly occupied regime, the electron-electron interaction is fully considered in Eq. (1). The solution for a certain impurity configuration is a very complicated many-body problem, which aims to determinate the occupancy factors n_i that minimize the total energy E of the system. This energy can be given as a summation of single-site energies, as given by Eq. (1), i.e.,

$$E=\sum_{i\neq j}\frac{(1-n_i)(1-n_j)}{r_{ij}}-2\sum_{i,\nu}\frac{(1-n_i)}{r_{i\nu}}+\sum_i n_i E_L(z_i)\ . \tag{3}$$

Except for the last term, which makes the difference for the QW, approximate analytical solutions for the DOS can be found in the limits of small and large compensations.[19] Monte Carlo simulation seems to be the only method able to treat satisfactorily the whole range of compensation.

Equation (2) gives the expression for the energy in the effective-mass approximation. The first attempt to solve it was due to Bastard[15] who used a variational approach for the infinite well. Several improvements on his calculations have been published.[20] Examples are the consideration of the finite width and height of the well[21] and electron-phonon mass renormalization.[22] However, they represent, in general, only small corrections to Bastard's results, no more than 10% each, and partially cancel each other. Another correction is related to the compensation. It is the contribution of the depletion potential of the ionized impurities. This effect should, in principle, be considered in a self-consistent way, but a simple analysis shows that it will also be small in the light-doping limit.[23] In this work we ignore these effects and follow the Bastard method in the calculation of $E_L(z_i)$.

Our Monte Carlo simulation starts by randomly distributing N donors and kN acceptors inside a rectangular box of height L and square basis of length $l=\sqrt{N}/n_d$. We fix n_d and, by increasing N, we increase the size of the sample. In order to find the distribution of the $(1-k)N$ uncompensated electrons over the donors, which minimizes the total energy, we follow the method of BEGS (Ref. 8). After the original purpose of investigating the occurrence of a Coulomb gap, this method has been widely used in different problems and by different groups.[1,3,10,24–30] The algorithm is very well described in Refs. 2, 18, and 26. The major feature of the method is that it provides ground states, or else, pseudo-ground-states, whose energies increase with any one-electron transition. They are pseudo-ground-states in the sense that, besides being tested only with single electron transitions, they are reached from a random initial configuration of the electrons. We did not look for the initial configuration which gives the lowest energy. This approximation has been widely used, not only because finding the true ground state is very time consuming, but also because the resulting DOS was shown to be very accurate. We also agree that, as pointed out by Davis, Lee, and Rice,[26] these psuedo-ground-states may be those of physical interest.

We used N up to 800 to simulate the system with $k=0.01$, 0.1, 0.3, 0.5, 0.7, and 0.9; $L=1$, 2, 3, and $4a^*$; $a^*\simeq 98$ Å for the $Ga_{1-x}Al_xAs/GaAs$ QW and $n_d=10^8$ cm^{-2} and 10^{10} cm^{-2}. The mean interimpurity distances in these cases are, respectively, 100 and 10 times larger than a^*. In these situations we always have $l>L$. It indicates that the finite size effect will be considerably smaller here than in the bulk semiconductor case.[1] The fraction of impurities near the boundaries is much bigger in the latter case. Therefore, we may conclude that the size effect can be neglected for $N=800$. In fact, our results changed very little when N changed from 400 to 800. All results shown in the next section are averages of 30 realizations (impurity configurations) with $N=800$.

III. RESULTS

A. The single-particle DOS

We emphasize that the DOS we have obtained is the one for adding or removing an electron without permitting relaxation. This DOS is constructed, after finding the pseudo-ground-state, by counting the number of donor states with energies given by Eq. (1), per unit energy interval, and averaging the results of several states of different impurity configurations. Following BEGS (Ref. 8) we have constructed the DOS using both kinds of averages, the simple and the μ average (μ meaning the pinning of the Fermi level). As occurred in their results, we found indistinguishable DOS for energies away from the Coulomb gap. The fluctuation of the Fermi level of the different realizations smooths out the Coulomb gap in the simple average. The vicinity of the Fermi level is well described only by the μ average.

The obtained DOS are shown, in atomic units, in Figs. 2, 4, 5, and 6. The energies are measured from $E_L(0)$, and therefore the unperturbed first subband starts at the energy which corresponds to the binding energy of an on-center impurity in a QW of width L. For $L=1a^*$, for example, it is ~ 2.3 Ry*. The figures show solid curves from which the histograms never deviate more than 10%. The histograms were made with 50 large intervals of energy and a much finer division (~ 20 times more) for the μ average in the vicinity of the Fermi level in order to achieve the same precision in the Coulomb gap description.

In Fig. 2 we show the dependence of the DOS on the

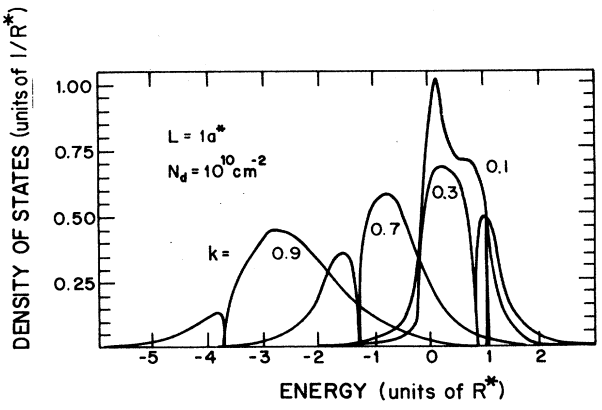

FIG. 2. DOS for an n-type lightly doped QW showing the effect of compensation.

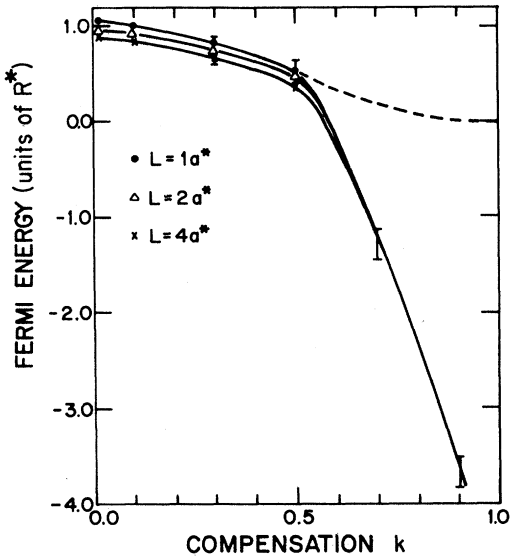

FIG. 3. The Fermi level as a function of the degree of compensation k for three values of the well width. Solid lines correspond to $n_d = 10^{10}$ cm^{-2} and the dashed line gives the behavior at low concentration limit.

degree of compensation for a typical QW of $L = 1a^*$ and $n_d = 10^{10}$ cm^{-2}. The dip in the DOS lies at the Fermi level and corresponds to the Coulomb gap. As the compensation increases, the tails, induced by disorder, increase and the whole band moves into a lower energy region, increasing the activation energy. With nonzero compensation the electrons are permitted to occupy donors preferably around the center of the well in order to minimize the total energy of the system. That is why the double-peaked structure of occupied states disappears for not too low compensation ($k > 0.1$).

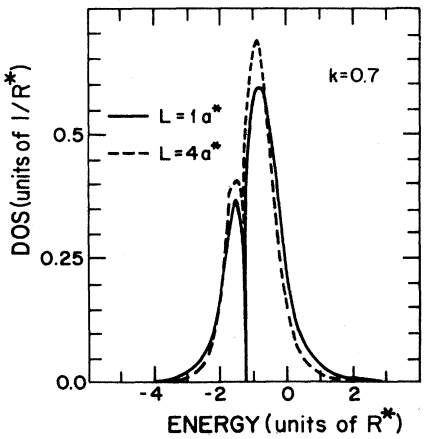

FIG. 4. Effect of the QW width on the DOS: the calculations were performed with $n_d = 10^{10}$ cm^{-2} for the two indicated values of L.

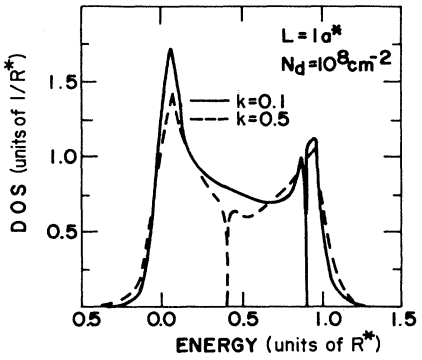

FIG. 5. DOS of lightly doped and compensated QW's in the very low impurity concentration regime.

The Fermi level is taken as the average of the energies of the lowest empty and highest occupied donor states. We have plotted in Fig. 3 the obtained averaged values, with their fluctuations shown as errors bars, as a function of compensation. The solid lines correspond to $n_d = 10^{10}$ cm^{-2}. We see that the Fermi level depends very weakly on the well width L. Only at small compensations does it make a small difference. This occurs as a general feature, i.e., the impurity band structure of lightly doped QW's is quite unsensible to the well width L at least in the range of $L = 1$ to $4a^*$. Figure 4 gives an example of a compensation of the DOS's. Similar to 3D systems, we observed that the Fermi level in the QW always decreases with compensation. The dashed line in Fig. 3 represents the low-concentration limit.

In the extremely dilute limit the Coulomb fluctuations become negligible and the DOS is unperturbed. In that case the degree of compensation determines only the position of the Fermi level. In this limit we have $E_F \to E_L(0)$ (zero in the figures) as $k \to 1$. As shown in Fig. 5, we found that the impurity concentrations corresponding to $n_d \leq 10^8$ cm^{-2} may be considered in this limit. The mean Coulomb energy $2\sqrt{n_d}$ Ry* is only 2% of the uncompensated spread of energy when $n_d = 10^8$ cm^{-2}.

Investigations of the low compensation limit, Fig. 6,

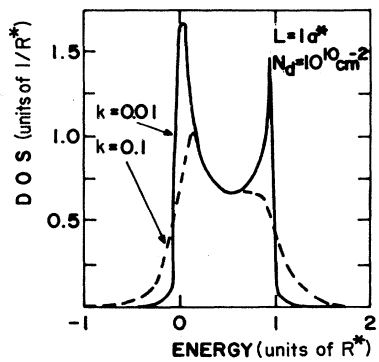

FIG. 6. The DOS for very small compensations.

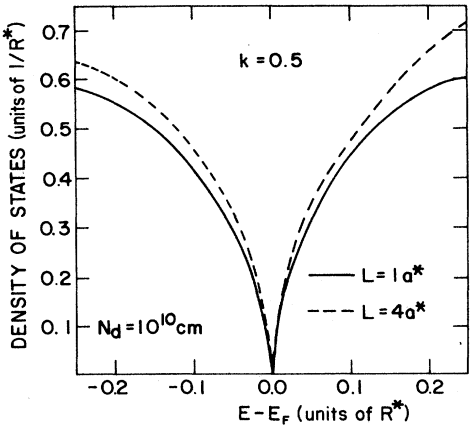

FIG. 7. Detail of the DOS for $k=0.5$, near the Fermi level. The Coulomb gap here, as in all other combinations of k, L, and n_d studied, appears close to a behavior in a first power on $E-E_F$.

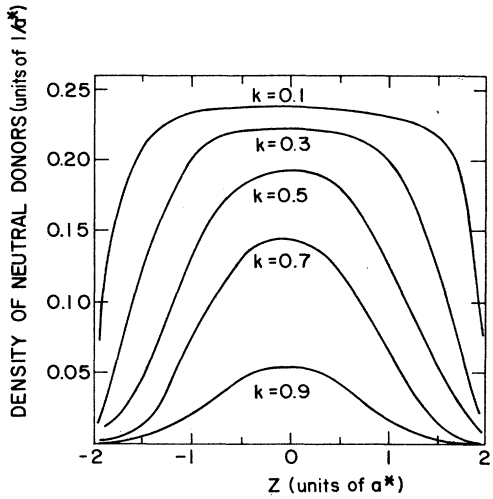

FIG. 9. Density of neutral donors inside the QW along the growth direction for different degrees of compensation. $n_d=10^{10}$ cm^{-2} and the curves are normalized to $1-k$.

show good agreement with uncompensated results. The Coulomb gaps in Fig. 6 were omitted for clarity.

The Coulomb gap was observed in all μ-averaged DOS's. Figures 7 and 8 show, in detail, examples of its occurrence. As mentioned, the curves present a maximum error of 10%. Our results clearly point to a $D(E)\propto|E-E_F|$ behavior for the DOS in the vicinity of the Fermi level. In accordance with the theory of ES,[9] we conclude that in the well-width range studied here, the bound electron system presents a two-dimensional character.

B. The charge distribution

Compensation permits the neutral donors to accumulate around the center of the well. Most experimental information about pure semiconductors and quantum wells at low temperatures comes from neutral-donor response. The properties of the latter depend first of all on their positions along the growth direction. The knowledge of their distribution is, therefore, very important.

After finding the pseudo-ground-state for each realization, we selected the neutral donors and distributed them among intervals in the z axis in accordance with their z coordinate. The histograms generated are shown smoothed out in Figs. 9 and 10. We used 50 intervals and the histograms did not deviate more than 5% from the curves. We have plotted the density of neutral donors per donor, so the distributions are normalized to $1-k$.

In Fig. 9 we show how the distribution varies with the degree of compensation. We see that the number of neutral donors in the proximity of the interfaces ($|z|\simeq L/2$) is always very small for finite compensations. As the

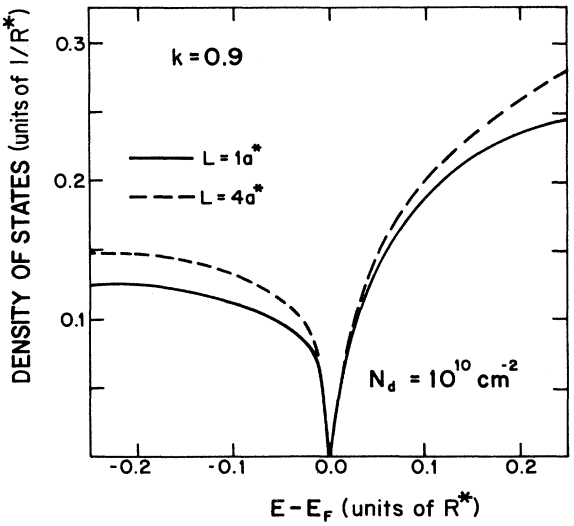

FIG. 8. Same as in Fig. 7 for $k=0.9$.

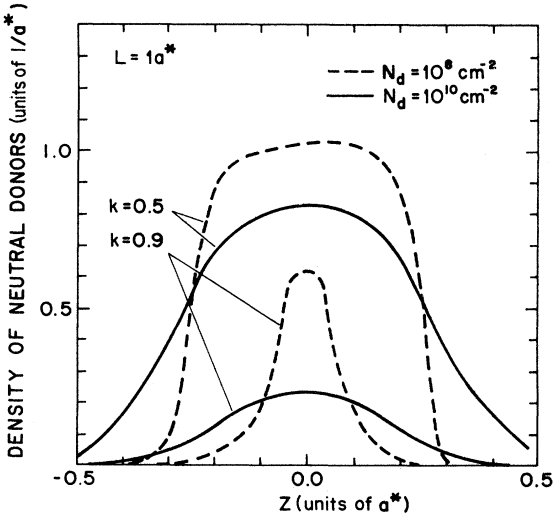

FIG. 10. Dependence of the neutral-donor distribution on both compensation and impurity concentration.

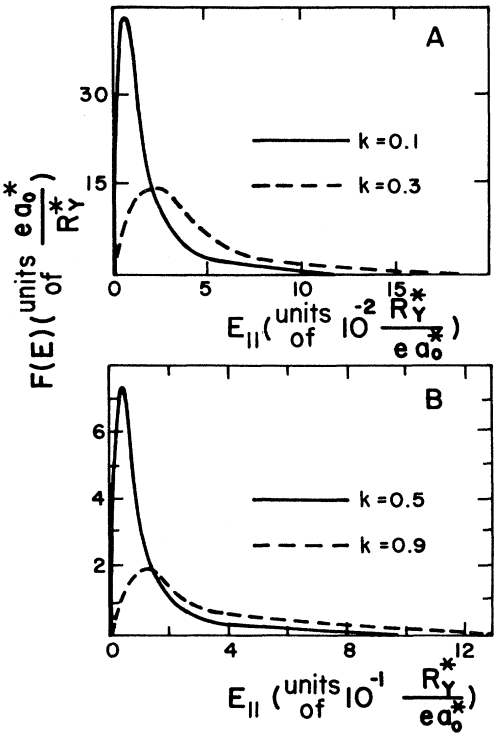

FIG. 11. Distribution of $E_{\parallel}$ for different values of compensation with $L = 1a^*$ and $n_d = 10^{10}$ cm^{-2}.

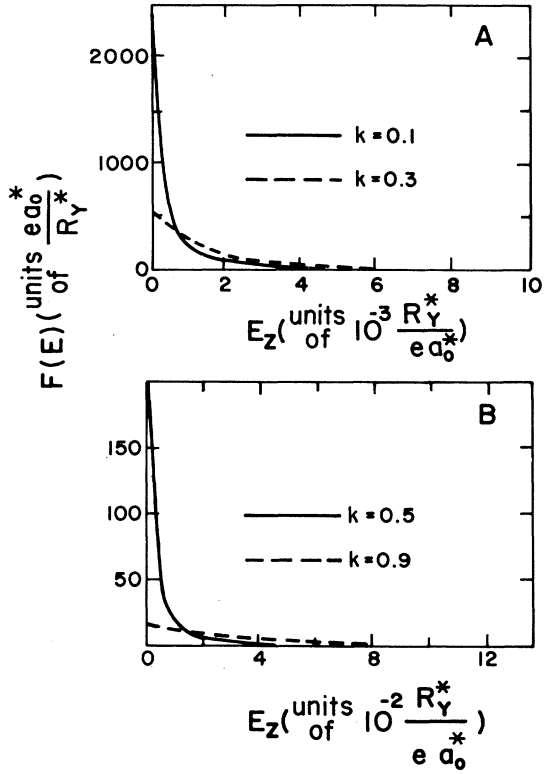

FIG. 12. Same as above for $E_{\perp}$.

compensation increases, the neutral donors accumulate more and more near the center of the well. The distribution width at half maximum is a function of the compensation. This function can be obtained numerically as described in this work and, therefore, be used to determine the degree of compensation of lightly doped QW's.

The dependence of the distribution of neutral donors on the impurity concentration can be understood from Fig. 10. As n_d decreases, the decreasing fluctuations on the Coulomb interactions make the change on the charge density close to the boundary between ionized and neutral donors sharper. The decay rate of the distribution is, then, a measure of n_d. This fact can also be used in the characterization of pure QW's.

C. Electric-field distribution at neutral-donor sites

For completeness we also investigated the electric field at neutral-donor sites. The static electric field produced by the ionized impurities causes a Stark shift and a splitting of the neutral-donors electronic levels. The field varies from donor to donor. Much attention has been given to the broadening of the intra-impurity absorption line due to this Stark effect.[3,4,30] The main difficulty in this problem is the calculation of the distribution of the electric field (and its square and derivations) at neutral-donor sites. Again, a Monte Carlo simulation method must be used in this problem for a proper treatment of the disorder.[4]

The electric field at the donor i, in units of Ry$^*/ea^*$, is given by

$$\mathbf{E}_i = -2\sum_{j=1}^{N}(1-n_j)\frac{\mathbf{r}_{ij}}{r_{ij}^3} + 2\sum_{\nu=1}^{kN}\frac{\mathbf{r}_{i\nu}}{r_{i\nu}^3}\ . \tag{4}$$

Its distribution function $F(E)$ is obtained by constructing the histograms exactly in the same way as was done for the DOS and charge distribution. The results we obtained are shown in Figs. 11 and 12. The fluctuations around the presented solid curves increase with compensation but are always negligible.

In Figs. 11 and 12 we show, respectively, the distributions of the absolute values of the components parallel and perpendicular to the interfaces. The well width and impurity concentration used were $1a^*$ and 10^{10} cm^{-2}, respectively. Firstly, we can see that, in fact, the z component is very small. It is, in general, 100 times smaller than the parallel component. The most likely z component is always zero. The xy component has a broader distribution and, as occurs in 3D systems,[26] the most likely value increases with compensation. The observed variation in the QW is much bigger than in 3D systems,[26] which is attributed to the low dimensionality of the QW.

The mentioned Stark broadening of spectral lines has been examined in the case of hydrogenic impurities in lightly doped bulk semiconductors.[3,30,31] A similar study for the QW case demands a calculation of the expressions for the level splitting in the presence of the confining potential.

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