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Self-consistent calculation of the electronic properties of a selectively doped $Al_xGa_{1-x}As$-GaAs quantum well under high magnetic fields

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We present a self-consistent calculation of the electronic structure of an $Al_xGa_{1-x}As$-GaAs-$Al_xGa_{1-x}As$ selectively doped single quantum well (QW) 500 Å wide under a high magnetic field applied perpendicular to the interfaces of confinement of the two-dimensional electron gas (2D EG). The calculation shows that the energy difference between electronic subbands changes with the magnetic field when three electronic subbands are occupied. This effect is related to the heterostructure character of the QW considered. Moreover, it is shown that these variations are related to the oscillatory behavior of the 2D EG's charge density. Our results seem to be confirmed by the available experimental data found in the literature, and we propose additional experiments in order to further verify the results obtained.

The two-dimensional electron gas (2D EG) formed in inversion layers, heterojunctions, or superlattices exhibits many interesting properties when subjected to magnetic fields. Quantum Hall effect[1] (QHE) and Shubnikov-de Haas (SdH) oscillations[2] are two of the most exciting properties under research. In this Rapid Communication, we address the problem of the effects produced on the electronic properties by a magnetic field B applied perpendicular to the plane of confinement of the 2D EG. We will show how the field affects the behavior of the electrons not only in the perpendicular direction to B but also in the parallel one. In particular, we have studied the case of a selectively doped double heterojunction system at two different 2D EG concentrations 10×10^{11} cm^{-2} and 15×10^{11} cm^{-2}, so that at $B=0$ two or three electric subbands are occupied, respectively. Our results show that the energy difference between subbands changes with B, which also varies the electron concentration (N_s) inside the well as a consequence of the self-consistent procedure. Furthermore, the change of N_s with the magnetic field is oscillatory. Baraff and Tsui[3] claimed that these charge oscillations are responsible for the QHE in agreement with a recent calculation[4] and measurement.[5] However, this paper is not concerned with the discussion about whether or not this oscillatory behavior is responsible for the plateaus of the QHE.[6] We will analyze the implications of this calculation in the measurements of the SdH oscillations and Raman scattering experiments in order to check if under a high magnetic field charge oscillations and, therefore, subband shifts are real facts. Following this goal, we will show an experimental result found in the literature that could support this model.

The schematic illustration of the conduction-band edge of a symmetrical selectively doped quantum well (QW) is shown in Fig. 1. It is convenient to introduce the method with the equations for the magnetic field applied in the z direction. In the effective mass approximation the Schrödinger equation to be solved includes the vector potential $\mathbf{A}$ for a uniform magnetic field in the z direction, and the electronic potential $V(z)$. Then, the total energy of the Landau levels (LL) is

$$E_{m,n}=E_m+(n+\tfrac{1}{2})\hbar\omega_c \ ,$$

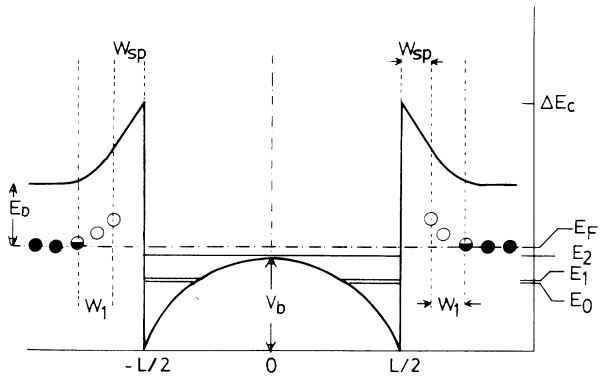

FIG. 1. Schematic diagram of the conduction-band edge for a selectively doped $Al_xGa_{1-x}As$-GaAs-$Al_xGa_{1-x}As$ quantum well.

where E_m are the subband energies determined by the one-dimensional Schrödinger equation for the wave function $\chi_m(z)$,

$$\left[\frac{h^2}{2m^*}\frac{d^2}{dz^2}+V(z)\right]\chi_m(z)=E_m\chi_m(z)\ . \tag{1}$$

The charge density which appears in the Poisson equation is

$$n(z)=-eN_L\sum_m\sum_n f(E_F-(n+\tfrac{1}{2})\hbar\omega_c-E_m)\times\chi_m^2(z)-\rho(z)\ , \tag{2}$$

where $N_L=2eB/h=4.836\times10^{10}$ and $B(T)$ is the number of carriers per LL. The function $f(E_F-E)$ is the fractional occupation of the state of energy E. We consider zero-temperature limit, so that $f=1$ for $E_F>E$, $f=0$ if $E_F<E$, and for $E_F=E$, f is allowed to take any value between zero and one in order to get consistency for the Fermi energy. Finally, $\rho(z)$ is the impurity density. In the doped region $\rho(z)=-eN_D$, where N_D is the donor concentration. Inside the QW, $\rho(z)=eN_I$, where N_I is the acceptor concentration.

We work in a Hartree approach, so that the effective $V(z)$ appearing in the Schrödinger equation is just the electrostatic potential $U(z)$. By solving simultaneously (1) and the Poisson equation we get $n(z)$, $E_{m,n}$, and N_s for each value of the magnetic field. In order to do that, we used a set of cubic-spline basis functions.[7] The Fermi level is then determined as described in Ref. 8. From E_F a new potential $V(z)$ is obtained. These steps are repeated until $V(z)$ converges.

We carried out the self-consistent calculation for a single quantum well as in Fig. 1 with the parameters $L_z=500$ Å, $W_{sp}=100$ Å. The conduction-band discontinuity for GaAs-$Al_xGa_{1-x}As$ ($x=0.3$) has been taken and $\Delta E_c=300$ meV. With respect to the binding energy of donors (E_D), these samples used to be Si doped and the activation energy of the Si-donor level is a controversial matter under current research.[9] Following Inoue, Sakaki, Yoshino, and Hotta[8] we have taken $E_D=96$ meV for $x=0.3$. The effect of the magnetic field on the binding energy can be very important for shallow donors, as has been shown by Poehler[10] in GaAs, but one can expect that this effect should be much less important for deep donors. Therefore, we have assumed that the binding energy E_D does not change with the magnetic field. We have taken a donor concentration in the $Ga_xAl_{1-x}As$ layer of $N_I=2.5\times10^{18}$ cm^{-3}, and we worked at two different impurities concentrations in the GaAs well in order to have two or three subbands occupied. For $N_I=5\times10^{17}$ cm^{-3} we get $N_s=10.3\times10^{11}$ cm^{-2} in the well and two occupied subbands, and for $N_I=5\times10^{14}$ cm^{-2} we have $N_s=14.7\times10^{11}$ cm^{-2} and three subbands occupied. The origin of energies, as shown in Fig. 1, is taken at the bottom of the well. The results obtained for the energy difference between subbands agree fairly well with Raman experiments by intersubband scattering on multiple modulation-doped GaAs-$Al_xGa_{1-x}As$ quantum wells of $L_z=500$ Å and $N_s=15\times10^{11}$ cm^{-2} per well.[11] As the magnetic field is turned on, E_F oscillates with respect to the bottom of the band. Moreover, because the Fermi level coincides with the donor level, the oscillations of the Fermi level produced by the field induce charge oscillations in the quantum well. As a consequence of the charge variations inside the QW, the electric field at the interfaces changes and induces a shift of the electronic subbands E_0, E_1, and E_2 with respect to the chosen origin of energies. The case in which the E_2 subband is also populated at $B=0$ ($N_s=14.7\times10^{11}$ cm^{-2}) has special characteristics associated with the fact that the E_2 subband suffers by itself changes in its electronic population when the magnetic field increases. Let us discuss in detail the results obtained for this case. Figure 2(a) shows the self-consistent calculation of the energy of the LL coming from the E_0 (crosses) and the E_2 (open circles) subbands. The position of the LL's coming from the E_1 subband are not shown in order to avoid complicating the figure. The position of the Fermi energy (filled circles) at different magnetic fields is plotted in Fig. 2(b). Full lines in Figs. 2(a) and 2(b) are, respectively, the LL's and the oscillations of the Fermi energy calculated non-self-consistently by holding constant the 2D EG density. Notice how the $n=0$ LL coming from the E_2 subband does not follow a straight line; it experiences oscillations as a consequence of the energy oscillations of the electronic subband. At magnetic field higher than 15 T this LL follows a straight line shifted downwards with respect to the non-self-consistent line. This behavior can be explained because for $B>15$ T the E_2 subband is completely depopulated [see Fig. 2(b)]. The shifts of the $E_{0,1}$ subbands are not so

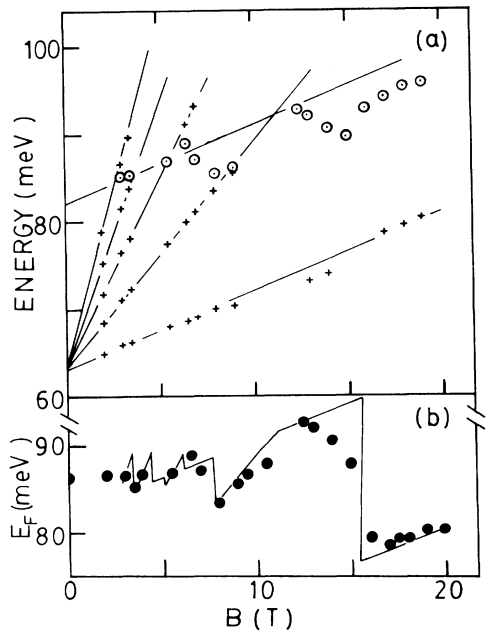

FIG. 2. (a) Landau levels coming from the E_0 (crosses) and E_2 (circles) electric subbands as a function of the magnetic field. (b) Behavior of the Fermi energy with B (filled circles). The full lines in both figures are the corresponding quantities calculated with a non-self-consistent method (see text).

large because they are confined in the triangular parts of the QW, they have heterostructure character [see Fig. 3(a)]. Contrarily, the E_2 subband is spread in the whole QW and it is roughly pinned at about 3 meV above the value of the band bending V_b that changes with B. In Fig. 3(b) the energy difference E_2-E_0 is plotted as a function of the magnetic field. This energy difference mainly oscillates as a consequence of the oscillations of the E_2 subband, and saturates at 15 T at a value of 16 meV. Let us remark that this effect is the general consequence of the fact that $E_{0,1}$ subbands have a heterostructure character and the E_2 subband has a QW character. Figure 4(a) shows the self-consistent results for N_s at different magnetic fields. By comparing Figs. 2 and 4(a) one observes that maxima in the Fermi energy correspond to minima in the values of N_s. This is so because the Fermi energy coincides with the donor energy and, therefore, an increase of E_F corresponds to a decrease of the width of the depletion layer in the doped region and, consequently, N_s would also decrease. Notice that the sawtooth behavior is not so sharp as in the case of $N_s=10.3\times10^{11}$ cm^{-2}, shown in Fig. 4(b), where only two subbands are occupied at 0 T. The existence of E_2 below E_F smoothes the oscillations of N_s due to two effects. In the first place, the presence of electrons in the E_2 subband reduces the jumps of E_F [see Fig. 2(b)]. In the second place, the self-consistent modification of the potential profile, associated with the rearrangement of charge, shifts the E_2 subband energy. As a consequence of this later effect, we found that, contrary to the case of $N_s=10.3\times10^{11}$ cm^{-2}, when E_F lies in the $n=0$ LL of the E_2 subband, the charge inside the QW does not decrease when B increases. In particular, in the region from 12 to 14 T the charge increases.

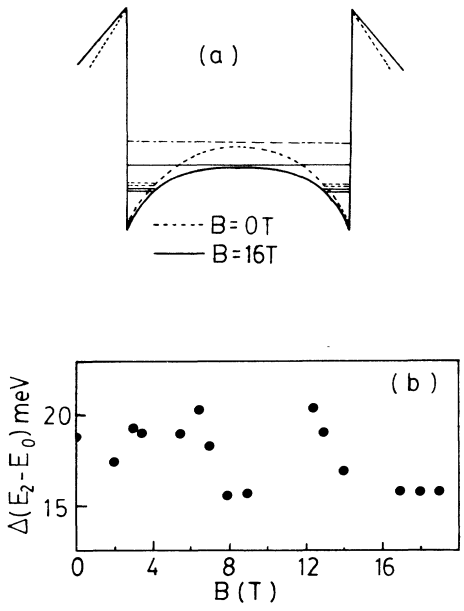

FIG. 3. (a) Effective potential $V(z)$ and the electric subbands E_n calculated at $B=0$ (full line), and $b=16$ T (broken line). (b) Behavior of the energy difference E_2-E_0 with B.

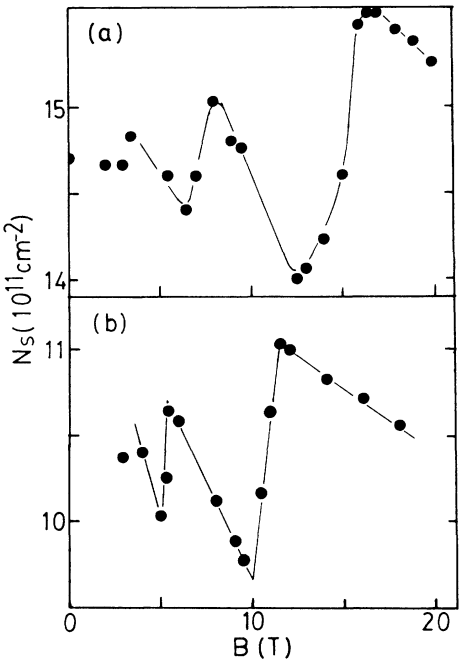

FIG. 4. Behavior of the electronic charge density N_s inside the QW as a function of the magnetic field B for the case of three [part (a)], and two [part (b)] subbands occupied at $B=0$. The full line is a guide for the eye.

Recently, Nizhankovskii, Mokerov, Medvedev, and Shadin[5] have detected oscillations of the chemical potential in 2D EG of GaAs-$Al_xGa_{1-x}As$ heterojunctions, and they claimed that these oscillations are related to charge oscillations. As far as we know, our results could be checked in two kinds of experiments: magnetotransport and light scattering in 2D EG. With respect to the magnetotransport experiments, the shifts of the electronic subbands will induce shifts in the minima of the SdH oscillations. But we have to stress the necessity that at least two subbands in heterojunctions or three in QW's (with heterostructure character) have to be occupied in order to enhance those observable shifts. In this way, Portal *et al.* [12] have reported SdH oscillations on GaInAs-AlInAs heterojunctions with two occupied subbands. It can be observed in Fig. 2 of Ref. 12 how the minima of the SdH oscillations are shifted with respect to the position at which they would be observable if the charge density were constant. Moreover, because the minima should correspond to jumps of the Fermi energy between LL's, it is possible to calculate the number of electrons N_s in the heterojunction at the fields where these minima appear. N_s at each minimum should be an integer or half integer times $2eB/h$ (not taking into account spin splitting). In Fig. 5 we present the results for N_s obtained from the data of Ref. 12. It is shown that N_s oscillates with the magnetic field. Of course, the direct comparison with our calculation is not possible due to the differences between the systems. Nevertheless, experiments like SdH oscillations have limitations because N_s can be only determined at certain values of B where minima in SdH appear.

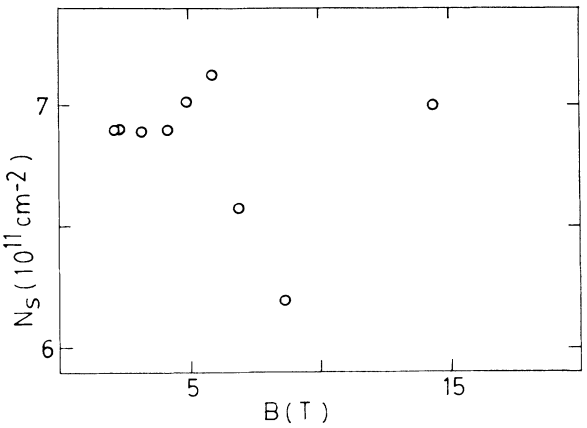

FIG. 5. Behavior of N_s with B obtained (see text) from the data shown in Fig. 1 of Ref. 12.

An experiment that could establish the reality of the charge oscillations is Raman scattering by intersubband levels under magnetic field. With this technique one can measure energy differences between subbands,[13] and therefore check whether the magnetic field affects the electronic subband energies and charge oscillations. Experiments of luminescence also seem to be a useful tool in order to detect the subband shifts.[11,14,15] However, the interpretation of the measurements can be difficult due to many different effects appearing in this kind of experiment, for example, band mixing in the valence band or luminescence coming out from impurities.

In summary, we have performed a self-consistent calculation of the electronic properties of a 500-Å-wide modulation-doped $Al_xGa_{1-x}As$-GaAs-$Al_xGa_{1-x}As$ QW. We have found good agreement with Raman experiments at B equal to zero. For external magnetic field perpendicular to the 2D EG, our results support the existence of charge oscillation between the QW and the doped region. The magnetic field also sensibly changes the energy difference between subbands due to the different characters of the $E_{0,1}$ (heterostructure) and the E_2 (QW) subbands. These results seem to be confirmed by experimental data found in the literature performed in systems similar to ours. Moreover, arguments are given in order to stress that experimental measurements of magnetotransport and Raman scattering could be useful tools in order to demonstrate those effects.

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