Magnetic-field-dependent self-consistent electronic structure of an inversion layer in the two-subband state

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An electron inversion layer with two populated electric subbands at zero magnetic field is considered in a perpendicular quantizing magnetic field. The band bending in the direction of the magnetic field depends on the latter via the occupation of the Landau levels according to their ordering and to their degeneration. Full self-consistent calculations are performed taking properly into account this effect for the first time. It is shown that qualitatively new features of the Landau-level spectrum and of the subband occupation appear. Most important is the occurrence of finite magnetic field regions where two Landau levels coincide and where both of these levels are partially occupied.

I. INTRODUCTION

Transport properties of the quasi-two-dimensional (Q2D) electron gas in inversion layers are of importance for fundamental research as well as for technical applications.[1,2] The magnetotransport measurements especially yield much information on the electronic nature of Q2D systems.[3] Therefore the energy spectrum of such systems in perpendicular magnetic fields is of special interest.

In recent years an increasing number of results concerning the electronic structure of inversion layers in magnetic fields were published where the influence of such semiconductor characteristics as nonparabolicity, band mixing, or impurity scattering were discussed.[4] But up to now, to our knowledge, besides our preliminary results,[5] there exists only one Landau-level (LL) calculation[6] considering the magnetic field in a self-consistent way.

In this paper we present full self-consistent calculations of the LL's for a Q2D electron gas with more than one occupied electric subband and show that several qualitatively new features of the LL spectrum occur. The most interesting new property is that a coincidence of two partially occupied LL's appears in various finite regions of the magnetic field.

II. FORMULATION OF THE PROBLEM

The system investigated is the symmetric potential (position-dependent conduction-band edge) caused by a δ sheet of a fixed positive charge per unit area N_T (as a model for δ doping layers[7] or grain boundaries[8]), negatively charged acceptors in the depletion layer (density N_{A^-}), and the inversion electrons (see Fig. 1). To demonstrate the main effect, nonparabolicity of the conduction band, spin splitting, and the influence of band-mixing effects are omitted. The calculations are done for temperature $T\rightarrow 0$ K. Parameters like effective mass m^* or energy gap E_g are chosen according to conditions in p-type InSb.

If a magnetic field B is applied parallel to the z direction (perpendicular to the Q2D electron gas), for a parabolic band in the effective-mass approximation, the Schrödinger equation separates into an equation for the motion in the (x,y) plane and the equation for the envelope wave functions $\chi_i(z)$:

$$\frac{1}{2m^*}\left[\left[-i\hbar\frac{\partial}{\partial x}+eBy\right]^2+\left[-i\hbar\frac{\partial}{\partial y}\right]^2\right]\phi_{lk_x}(x,y) = E_l\phi_{lk_x}(x,y)\ , \quad (1)$$

$$\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2}+V(z)\right]\chi_i(z)=E_i\chi_i(z)\ . \quad (2)$$

[An asymmetric gauge was assumed for the vector potential $\mathbf{A}=(-By,0,0)$.] The energy spectrum reads as

$$E_{il}=E_i+E_l = E_i+\hbar\omega_c(l+\tfrac{1}{2})\ , \quad \omega_c=eB/m^*,\quad i,l=0,1,2,\ldots \quad (3)$$

E_i being the subband energies and l the Landau quantum number. (As usual in the determination of the E_{il}, their broadening due to disorder, scattering, etc. is omitted.) Simultaneously all charges have to satisfy Poisson's equation

$$\frac{d^2}{dz^2}V(z)=-\frac{e^2}{\epsilon_r\epsilon_0}[n(z)+N_{A^-}\Theta(d-|z|)-N_T\delta(z)]\ , \quad V(|z|=d)=E_c,\quad V'(|z|=d)=0\ . \quad (4)$$

The following parameters are used:[8] $E_g=235.2$ meV, $m^*=0.0155m_e$, $\epsilon_r=17.4$, $N_{A^-}=5\times10^{15}$ cm^{-3} for $|z|<d$, and $N_{A^-}=0$ for $|z|\geq d$. For $T\rightarrow 0$ the acceptors are ionized over the space charge width $2d$, which has to be determined in the self-consistent cycle. The difference between conduction-band edge E_c and the Fermi energy

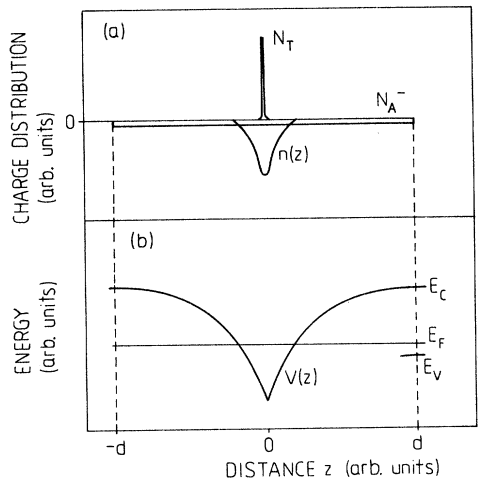

FIG. 1. Schematic representation of the system investigated. (a) Charge distribution, consisting of a δ sheet of a fixed positive charge N_T, negatively charged acceptors N_{A^-} in the depletion layer $2d$, and the inversion electrons $n(z)$. (b) The symmetric potential caused by the charge distribution shown in (a).

E_F in the bulk equals $E_c - E_F = 234.9$ meV, and there its magnetic field dependence is neglected. Throughout the calculations E_F was defined as the zero of the energy scale: $E_F = 0$. The density of the positive charges N_T is assumed as a fixed quantity reflecting the real conditions in δ doping layers or grain boundaries. We chose $N_T = 0.72 \times 10^{12}$ cm^{-2} to have two occupied subbands for zero magnetic field. Corresponding to the boundary conditions in (4) we set $\chi_i(|z| \geq d) = 0$ in the numerical calculations. This assumption causes an error for the subband energies less than 0.01%.

The eigenfunctions of the decoupled three-dimensional Schrödinger equation [Eqs. (1) and (2)] in an infinite Q2D system,

$$\psi_{ilk_x}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} \chi_i(z) e^{ik_x x} f_{lk_x}(y) ,$$
$$f_{lk_x}(y) = \left[\frac{m^* \omega_c}{\hbar}\right]^{1/4} (2^l l! \sqrt{\pi})^{-1/2} \times \exp\left[-\frac{m^* \omega_c}{2\hbar}\left[y + \frac{\hbar k_x}{eB}\right]^2\right] \times H_l\left[\left[\frac{m^* \omega_c}{\hbar}\right]^{1/2}\left[y + \frac{\hbar k_x}{eB}\right]\right] \quad (5)$$

are normalized to $\delta_{ii'}\delta_{ll'}\delta(k_x - k_x')$. Consequently the eigenvalues are infinitely degenerate with respect to k_x. $H_l(\xi)$ are the Hermite polynomials.[9] The density of inversion electrons is given with (5) as

$$n(z) = 2 \sum_{i,l} \int_{-\infty}^{+\infty} dk_x \, f(E_{il}) |\psi_{ilk_x}(r)|^2 = \frac{2eB}{h} \sum_{i,l} f(E_{il}) |\chi_i(z)|^2 \quad (6)$$

with a spin-degeneracy factor 2 and with the Fermi-Dirac distribution function $f(E)$. In the second step in (6) the k_x integration yields the degeneracy factor eB/h according to the properties of the wave function (5). Indeed, the density depends only on z as already assumed in (4). The total inversion electron density per unit area is $n_s = \int_{-d}^{+d} dz \, n(z)$. For $T \to 0$ K all $f(E_{il})$ have the value 0 or 1 only for integer (M) filling factors $\nu = n_s/(2eB/h) = M$ determining the values $B^{(M)} = n_s h/2eM$ in the vicinity of which the number of occupied LL's is changed by one. For the magnetic field in the region between the $B^{(M)}$ (except level crossing, see below) one level $E_{i'l'}$ lies in the region $|E_{i'l'} - E_F| \lesssim k_B T \to 0$ and one has $0 < f(E_{i'l'}) < 1$ for this level. Therefore, it is convenient to write (6) as

$$n(z) = \frac{2eB}{h} \sum_i \nu_i |\chi_i(z)|^2 , \quad \sum_i \nu_i = \nu, \text{ one } \nu_i \text{ not integer} \quad (7)$$

where $\nu_i(B)$ is the filling factor of the ith subband and in general (except for $B^{(M)}$ and level crossing) one ν_i (for $i = i'$) is not integer, reflecting the partial occupation of this level which then practically coincides with the bulk Fermi energy.

According to (4) one has charge neutrality

$$N_T = n_s + 2N_{A^-} d . \quad (8)$$

The system of equations (2)–(4), (7), and (8) has to be solved numerically in a self-consistent manner with the magnetic field as the parameter. The $\nu_i(B)$ must be determined according to the ordering of the levels (3). Thus, most important is that according to (7) the charge distribution depends on the occupation of the LL's and hence on the magnetic field. But the charge distribution, in turn, determines the subband energies E_i and hence the LL's (3). In this way the electric subband energies E_i determined by (2) become magnetic field dependent via the occupation of the LL's although (2) is decoupled exactly from (1).

III. RESULTS AND DISCUSSION

Usually the calculations of the LL's (e.g., Refs. 8 and 10) were done non-self-consistently insofar as the spectrum (3) is used (eventually modified for nonparabolicity of the band structure) where the subband energies E_i are determined self-consistently but for zero magnetic field. Such calculations are often denoted as self-consistent ones[10] though they are not, as explained above. In Fig. 2 such a non-self-consistent scheme (solid lines) is compared with our full self-consistent results. [To compare our results with usual notations, we chose for the figures the potential bottom $V(z=0)$ as the energy zero.] For a better understanding at first, peculiarities of the non-self-consistent scheme are discussed. In this case n_s is fixed; the Fermi energy varies with one LL and jumps to the next one at the value $B^{(M)}$ as already discussed above. Furthermore, there are points where LL's belonging to

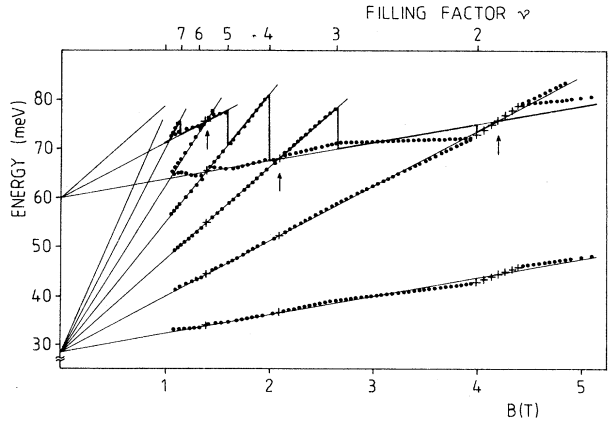

FIG. 2. Non-self-consistent (solid lines) and self-consistent results (points and crosses) for the LL scheme. Points are the solutions using Eqs. (2)–(4), (7), and (8), and the crosses are those using Eqs. (2)–(4), (8), and (9). The bold line represents the Fermi energy E_F in the non-self-consistent picture. Arrows show the crossing points where E_F changes from one LL to another without any jump.

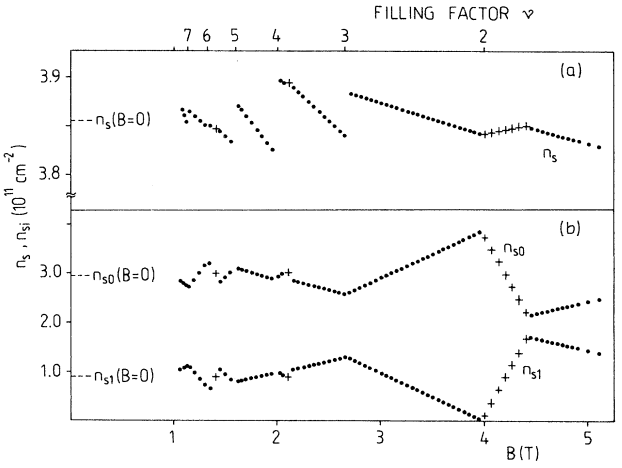

FIG. 3. Self-consistently calculated subband occupations n_{si} and total electron density n_s as functions of magnetic field B. Points and crosses as in Fig. 2.

different subbands cross each other (in Fig. 2 indicated by arrows). If one of them is partially occupied, the Fermi energy follows one level (belonging to the subband i) and changes then to the other LL (of the subband i') without any jump. But in this case a finite amount of charge is transferred from subband i to i' having different envelope functions and hence different spatial extensions.

Now let us look at the magnetic-field-dependent self-consistent results obtained as described in Sec. II. They are denoted by points. It is seen that the new dependence of the LL's on the magnetic field causes quantitative deviations from the non-self-consistent scheme up to $0.1\hbar\omega_c$ for higher magnetic fields. They decrease for smaller fields. At the "jumps" (ν integer) it is actually $V(z)$, not the Fermi energy, that is changed abruptly. More precisely, this happens in a very narrow region of the magnetic field, as will be shown in more detail in a subsequent paper.[11]

In Fig. 3 the subband occupations $n_{si}=2eB\nu_i/h$ and the total inversion electron density $n_s=\sum_i n_{si}$ are shown. The occupations are strongly dependent on B since in any case with increasing field due to the degeneration $2eB/h$ of the LL's, the number of electrons in a completely occupied LL increases. At the same time, the partially filled LL is depopulated. The total density n_s varies only slightly [charge exchange between inversion and depletion layer according to (8) with $N_T=$const]. The self-consistent calculation yields for high magnetic fields (only one LL occupied) an almost linear dependence of the density on the magnetic field with a slope $dn_s/dB\sim-2.2\times10^{-9}$ cm^{-2}T^{-1} (note that n_s itself is of the order 10^{11} cm^{-2}). An analytical estimate gives for this slope $-\hbar\epsilon_0\epsilon_r/(m^*ed)$ and with the parameters used here -2.1×10^9 cm^{-2}T^{-1}.[11]

Figure 4 shows the magnetic field dependence of the subband energies. Their behavior is closely connected with the magnetic field dependence of the subband occupations shown in Fig. 3. In dependence on the fact that the partially filled LL belongs to the one or the other subband, both subband energies [relative to $V(z=0,B)$] show the following behavior with increasing magnetic field: They either both decrease with decreasing separation or they both increase with increasing separation. Although, of course, this subband energies E_i arise only from the motion in the z direction they determine the whole spectrum according to (3). This results in a varying slope of the LL's E_{il} contrary to the non-self-consistent picture (cf. Fig. 2). In several regions of the magnetic field dE_i/dB exceeds $d(\hbar\omega_c/2)/dB$. Therefore, e.g., for $B\sim1.2$ T the LL E_{10} decreases with increasing magnetic field (also on the absolute scale with $E_F=$const as the energy zero).

Finally, let us look at the regions around the crossing

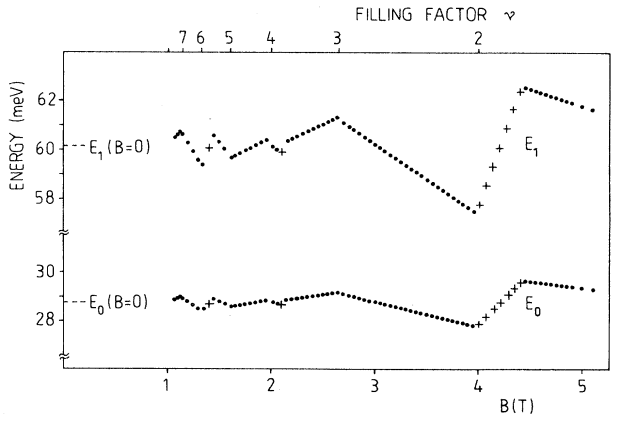

FIG. 4. Self-consistently calculated subband energies E_i (relative to the potential bottom) as functions of magnetic field B. Points and crosses as in Fig. 2.

points of the non-self-consistent scheme (indicated in Fig. 2 by arrows). It is seen that the partially filled level in the full self-consistent scheme approaches another one (filled or empty) for increasing magnetic field at some value B and at higher value for decreasing field. In the vicinity of this point there remains a finite interval of the magnetic field in which the self-consistent scheme as described in Sec. II has no solution. This was already predicted qualitatively by us.[12]

What actually happens is the following. For increasing B, the one partially occupied level (say $E_{i'l'}$) with $0<f(E_{i'l'})<1$ approaches another one ($E_{i''l''}$) which may be empty [$f(E_{i''l''})=0$] or completely filled [$f(E_{i''l''})=1$]. If the separation $|E_{i'l'}-E_{i''l''}|$ between these two levels becomes comparable to k_BT ($\rightarrow 0$), it is no longer justified to assume that only one level is occupied partially. Thus, in the B region in question, instead of (7) one has to use

$$n(z)=\frac{2eB}{h}\sum_i \nu_i|\chi_i(z)|^2 ,$$

$$\text{two } \nu_i \ (i=i',i'') \text{ not integer} \qquad (9)$$

and to take into account that for $T\rightarrow 0$ both these levels coincide with one another and with the Fermi energy: $E_{i'l'}=E_{i''l''}=E_F$. In the interval the partial occupation changes from one of these levels to the other one continuously. Numerically one has now to solve the system of equations (2)–(4), (8), and (9). Of course, in the self-consistent cycle one has to determine one quantity more than before, namely the second partial occupation. Indeed, one has also the additional condition of coinciding levels. The numerical solution is unique in this way. Results are indicated by crosses in Figs. 2–4. One sees the common level around the original crossing point and the transfer of charge from one subband to the other (n_{si}) connected with only a slight change of the total density n_s. It should be emphasized that the occurrence of a finite interval on the magnetic field scale where two levels for $T\rightarrow 0$ coincide is a qualitatively new feature of the spectrum.

We conclude that by properly taking into account the dependence of the occupation of the Landau levels on the magnetic field, one is led to new and interesting features of the self-consistently calculated electronic structure of inversion layers. For the first time this was demonstrated here for a symmetric potential. General considerations on this question will be published elsewhere.[11] The peculiarities concern the total electron density, the subband occupations, the subband energies, and the complete Landau-level spectrum. For the latter, most important is, in our opinion, the coincidence of two Landau levels and the partial occupation of both in finite magnetic-field regions.

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[1]T. Ando, A. B. Fowler, and F. Stern, Rev. Mod. Phys. **54**, 437 (1982).

[2]G. J. Iafrate, Phys. Scr. **T19**, 11 (1987).

[3]*High Magnetic Fields in Semiconductor Physics,* Vol. 71 of *Springer Series in Solid State Sciences,* edited by G. Landwehr (Springer, Berlin ,1987).

[4]See, e.g., E. Bangert and G. Landwehr, Surf. Sci. **170**, 593 (1986); U. Ekenberg and M. Altarelli, Phys. Rev. B **32**, 3712 (1985).

[5]S. Handschack, G. Paasch, and G. Gobsch, Phys. Status Solidi B **147**, K125 (1988).

[6]J. Sanchez-Dehesa, F. Meseguer, F. Borondo, and J. C. Maan, Phys. Rev. B **36**, 5070 (1987).

[7]For example, G. H. Döhler, Surf. Sci. **73**, 97 (1978).

[8]G. Gobsch, G. Paasch, and H. Uebensee, Phys. Status Solidi B **135**, 283 (1986).

[9]*Pocketbook of Mathematical Functions,* edited by M. Abramowitz and I. A. Stegun (Verlag Harri Deutsch, Thun, 1984).

[10]U. Merkt, M. Horst, T. Evelbauer, and J. P. Kotthaus, Phys. Rev. B **34**, 7234 (1986).

[11]G. Paasch, S. Trott, and G. Gobsch (unpublished).

[12]G. Paasch, D. Schulze, and G. Gobsch, in Proceedings of the 17th Symposium on Electronic Structure, TU Dresden, Dresden, 1987, edited by P. Ziesche (unpublished).