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LETTER TO THE EDITOR

Self-consistent electron subbands of GaAs/AlGaAs heterostructures in magnetic fields parallel to the interface

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Abstract. The effect of strong magnetic fields parallel to the GaAs/$Ga_xAl_{1-x}As$ interface on the subband structure of a 2D electron layer is investigated theoretically. A system with two levels occupied in zero magnetic field is considered and the magnetic-field-induced depletion of the second subband is studied. The confining potential and the electron energy dispersion relations are calculated self-consistently. The electron–electron interaction is taken into account in the Hartree approximation.

Recently, it was suggested [1] that deviations of the 2D Fermi lines from a circular shape, caused by the combined influence of an approximately triangular potential well and of the parallel magnetic field, may play an important role in the theory of magnetotransport in 2D inversion layers at interfaces of GaAs/$Al_xGa_{1-x}As$ heterostructures.

Zawadzki *et al* [2] theoretically studied Fermi lines of narrow-band-gap semiconductors of the In–Sb type. Their analysis was based on two main simplifications: (i) the confining potential $V_{conf}(z)$ was taken to be in the form of a triangular potential well and (ii) the interface was considered to be an impenetrable hard wall, which could be accounted for by an appropriate boundary condition for the wavefunction. In this model the spacing of levels due to the magnetic quantization is inversely proportional to the effective mass m, while the spacing of subbands due to the confining potential is proportional to $(1/m)^{1/3}$. Thus, for narrow-gap semiconductors with small effective masses the electric and magnetic effects become comparable for magnetic fields which are not too high, and for this range of fields a change of Fermi lines from the circular to the 'egg-like' form is also expected.

In semiconductors with larger effective mass, such as GaAs, the effect of a parallel magnetic field should be less pronounced and, therefore, up until now it had mainly been treated using perturbation theory [3]. On the other hand, it is well known that due to the small conduction band offset between GaAs and $Al_xGa_{1-x}As$ the interface wall is rather soft and electrons can partly penetrate into $Al_xGa_{1-x}As$. Thus, to obtain quantitatively better results, it is desirable to go beyond the triangular well approximation or the perturbation approach. For this reason we decided to perform the full numerical self-consistent study of the influence of the in-plane magnetic field on the subband shape of a 2D electron gas confined to the GaAs/$Al_xGa_{1-x}As$ interface and this letter presents our results.

It is now well established that the numerical self-consistent calculation based on the effective mass approximation correctly describes the observed electron subband structure in zero magnetic field. Moreover, generally accepted methods of such calculations, *including*

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the Hartree approximation, should be valid in the presence of the magnetic field as well as in the zero-field case. The self-consistency requirement, i.e. the requirement of solving coupled Poisson and Schrödinger equations, is an important aspect of the energy spectra calculations in doped heterostructures as the charge distribution reacts on the confining potential, which itself determines the charge distribution. In strong magnetic fields there is one more reason for the self-consistency: the charge redistribution caused by the magnetic field.

For doped GaAs/$Al_xGa_{1-x}As$ heterostructures the total charge density $\rho(z)$ entering the Poisson equation can be split into parts corresponding to concentrations of electrons, their parent donors in $Al_xGa_{1-x}As$, and ionized residual acceptors in GaAs

$$\rho(z) = e\left[N_e(z) - N_d^+(z) + N_a^-(z)\right]. \tag{1}$$

We accept the usual approximation of constant impurity concentrations and assume donors and acceptors to be ionized within certain finite intervals l_d and l_a: $N_d^+(z) = N_d$ for $-l_d - w \leqslant z \leqslant -w$ and $N_a^-(z) = N_a$ for $0 \leqslant z \leqslant l_a$; w is the spacer thickness (see figure 1). The confining potential

$$V_{conf}(z) = V_b(z) + V_{sc} \tag{2}$$

is a sum of the step function $V_b(z) = V_b\Theta(-z)$ corresponding to the conduction band discontinuity and of the Hartree term $V_{sc}(z)$ determined from the Poisson equation

$$\frac{d^2V_{sc}}{dz^2} = -\frac{\rho(z)}{\epsilon}. \tag{3}$$

The conduction band offset V_b and the dielectric constant ϵ enter our calculations as input parameters.

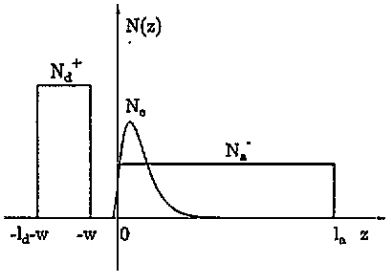

Figure 1. The charge distribution in a single modulation-doped GaAs/$Al_xGa_{1-x}As$ heterojunction with quasi-2DEG at the interface in the depletion length model.

The simplest semi-empirical model working quantitatively for the lowest conduction states of GaAs/$Al_xGa_{1-x}As$ heterostructures is used to solve the Schrödinger equation in the envelope function approximation. The envelope function is assumed to be built from host quantum states belonging to a single parabolic band. The effect of the effective mass mismatch is completely neglected and the envelope functions of GaAs and $Al_xGa_{1-x}As$ are smoothly matched at the interface.

Due to the translational invariance in the layer plane the wavefunction $\psi_\alpha(\boldsymbol{r})$ can be factorized

$$\psi_\alpha(\boldsymbol{r}) = \frac{1}{\sqrt{S}}e^{i(k_x x + k_y y)}\phi_{i,k_x}(z) \tag{4}$$

and the Schrödinger equation may be written as

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}+\frac{1}{2m}\left(\hbar k_x-|e|B_y z\right)^2-eV_{\mathrm{conf}}(z)\right]\phi_{i,k_x}(z)$$
$$=\left[E_i(k_x)-\frac{\hbar^2k_y^2}{2m}\right]\phi_{i,k_x}(z) \tag{5}$$

where the magnetic field parallel to the layer plane x–y has the form $\boldsymbol{B}\equiv(0, B_y, 0)$. As the heterostructure is in electric and thermodynamic equilibrium two additional conditions must be fulfilled: the charge balance condition and the constant chemical potential condition. For details about the self-consistent procedure for zero magnetic field (but relevant for $B\neq 0$ as well) we refer to works by Stern and Das Sarma [4] and Ando [5]. From the latter paper we also took values of the band offset $V_b = 300\,\mathrm{meV}$ and the dielectric constant $\epsilon = 12.9$.

To distinguish between the charge redistribution resulting from the standard self-consistent loop in zero magnetic field and changes due to the magnetic field we performed the self-consistent procedure in two steps. First, the electron structure was calculated self-consistently for $B = 0$ and $N_e(z)$ and V_{conf} obtained from this calculation were used as input values for the electron structure determined for $B\neq 0$. In this way the 'intermediate' results ($B\neq 0$, but self-consistency only for $B = 0$) were obtained. In the second step the procedure followed the full self-consistent calculation for $B\neq 0$ yielding the final results.

The parameters $N_d = 2\times 10^{18}\,\mathrm{cm}^{-3}$, $N_a = 10^{13}\,\mathrm{cm}^{-3}$ and $w = 2\,\mathrm{nm}$ were chosen to obtain the electron system of $N_e\approx 14\times 10^{11}\,\mathrm{cm}^{-2}$ having two levels occupied in zero magnetic field and depleting the second level at $\sim 10\,\mathrm{T}$. Note that in this case the 'intermediate' results are all based on the electron density corresponding to two occupied levels, while the full self-consistent study includes the magnetic-field-induced transfer of electrons from the second subband to the first one in the solution of coupled Poisson and Schrödinger equations.

In zero magnetic field the in-plane electron motion and its out-of-plane component along the z axis are completely independent. This means that all electrons within a subband are described by a single localized wavefunction $\phi_i(z)$ regardless of their energies $E_i(k_x)$ and wavevectors k_x, k_y. In our case, with two occupied subbands, we have two different wavefunctions; their centres of mass $\langle z\rangle_0$ and $\langle z\rangle_1$ determine the averaged distances of electrons in subbands from the interface.

When the magnetic field is applied the effective electro-magnetic potential V_{eff} composed from the harmonic magnetic potential and the confining potential V_{conf} is built

$$V_{\mathrm{eff}}=\frac{m\omega^2}{2}(z-z_0)^2-eV_{\mathrm{conf}}(z). \tag{6}$$

The centre z_0 of the magnetic part of the effective potential is related to the wavevector component k_x by $z_0=\hbar k_x/m\omega$. Thus the magnetic field couples the electron motion in the x and z directions and for each k_x a new $\phi_{i,k_x}(z)$ must be calculated. Also the energy spectrum $E_i(k_x)$ will deviate from the original parabolic dependence on k_x and $E_i(k_x)\neq E_i(-k_x)$ due to the breakdown of the time reversal symmetry. This results in the asymmetric Fermi lines. New eigenfunctions $\phi_{i,k_x}(z)$ are shifted from their original positions $\langle z\rangle_0$ and $\langle z\rangle_1$ obtained for $B = 0$ and, therefore, the charge distribution described by their squares is also changed.

There exists a relation between the centre of mass of the wavefunction $\phi_{i,k_x}(z)$ and the shape of the energy spectrum curve $E_i(k_x)$

$$\langle z\rangle_{i,k_x}=\frac{\hbar k_x}{m\omega}-\frac{1}{\hbar\omega}\frac{\partial E_i(k_x)}{\partial k_x} \tag{7}$$

which makes it possible to calculate this quantity without numerical difficulty. As there is a one-to-one correspondence between $\langle z\rangle_{i,k_x}$ and k_x, and as we are interested mainly in the charge redistribution induced by the in-plane magnetic field, figure 2 presents the energy subbands as functions of $\langle z\rangle_{i,k_x}$ instead of k_x, together with the shape of the self-consistent potential V_{conf}. The broken lines correspond to 'intermediate' results while the full lines describe the results of the full self-consistent calculations.

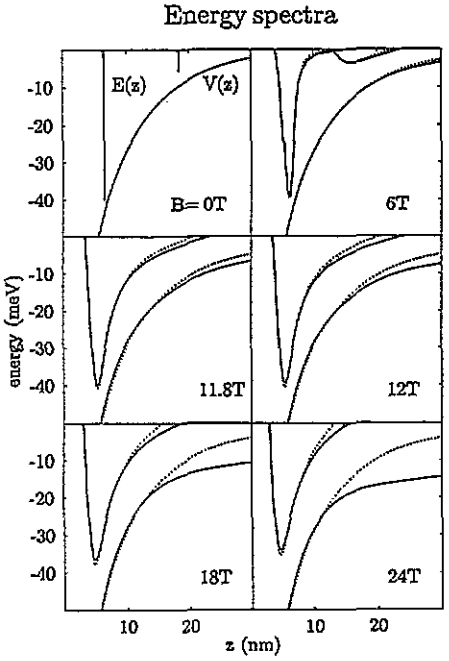

Figure 2. Electron eigen energies $E(z)$ calculated as functions of $\langle z\rangle_{i,k_x}$ and the confining potential $V(z)$. The energies are measured from the Fermi energy. Broken lines correspond to the 'intermediate' results, full lines to the results of the full self-consistent calculations.

We have already mentioned that in zero magnetic field electrons reach all possible energies for just two centres of mass $\langle z\rangle_0$ and $\langle z\rangle_1$. If magnetic field is applied the electrons with low energies remain localized approximately around these two values but the electrons with energies closer to the Fermi level are shifted either to the interface or deep into the bulk GaAs, depending on the direction of their motion. The minimum and maximum distances $\langle z\rangle_{i,k_x,\mathrm{min}}$ and $\langle z\rangle_{i,k_x,\mathrm{max}}$ are reached for the Fermi energy and correspond to electrons moving in opposite directions. Note that the velocity is related to the energy spectrum by

$$\langle v\rangle_{i,k_x} = \frac{1}{\hbar}\frac{\partial E_i(k_x)}{\partial k_x}. \tag{8}$$

The electrons in the second subband are more sensitive to the magnetic field and the second subband is emptied at $B = 11.8\,\mathrm{T}$ for 'intermediate' and at $B = 12\,\mathrm{T}$ for the full self-consistent calculation.

The difference between the two types of calculation increases with increasing magnetic field. This is particularly valid for depressions of the confining potential far from the interface which appear in results of full self-consistent calculations. Note that in spite of this the maximum distance of an electron from the interface is not reached for the maximum magnetic field, but approximately for $B = 12\,\mathrm{T}$.

Figure 3 shows the Fermi lines based both on 'intermediate' and full calculations. Two concentric circles correspond to two parabolic subbands in the zero magnetic field. With

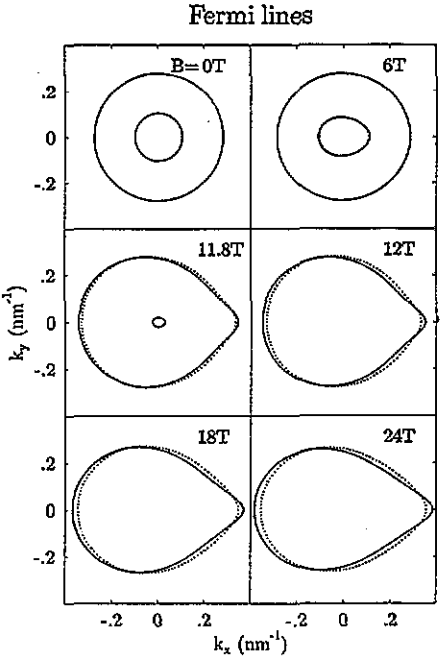

Figure 3. Lines of constant Fermi energi in (k_x, k_y) space are shown for the two-subband system depleting the second subband at 11.8 T ('intermediate' result) and 12 T (full self-consistent result). The distances in k-space are measured from their centres.

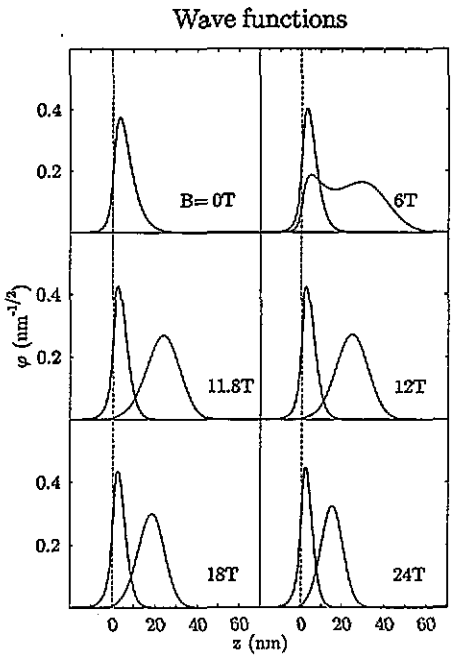

Figure 4. Wave functions of first-subband electrons with $\langle z\rangle_{0,k_x,\min}$, $\langle z\rangle_{0,k_x,\max}$ illustrating the charge redistribution due to in-plane magnetic fields.

increasing field the area of the second-subband Fermi surface decreases and the Fermi line of the first subband takes an 'egg-like' form. Its left half, corresponding to electrons close to the interface, remains approximately circular, while the right half, describing the electrons that move far from the interface in the bulk GaAs, takes a nearly parabolic form. The gross qualitative features of both 'intermediate' and full results are very similar. A closer look shows marked differences between the full and broken lines. Because of the large magnetic-field-induced charge redistribution, the full lines are qualitatively different having a 'pear-like' rather than an 'egg-like' shape.

Individual wavefunctions are influenced by the magnetic field to an even greater extent. Figure 4 shows the first-subband wavefunctions $\phi_{0,k_x}(z)$ corresponding to $\langle z\rangle_{0,k_x,\min}$ and $\langle z\rangle_{0,k_x,\max}$. In comparison with the case $B = 0$, the function corresponding to $\langle z\rangle_{0,k_x,\min}$ is narrower and shifted to the $Al_xGa_{1-x}As$ spacer and dotted region, while the function corresponding to $\langle z\rangle_{0,k_x,\max}$ is broad and almost entirely inside the bulk GaAs. Note the double-peak structure of the wavefunction for $B = 6$ T.

We conclude that, as in the case of zero magnetic field, the electron structure of $GaAs/Al_xGa_{1-x}As$ heterostructures in strong in-plane fields has to be calculated self-consistently if we are interested in semi-quantitative results. Both the energy spectra and the confining potential are affected by the charge redistribution caused by the magnetic field. On the other hand the total number of electrons remains constant. This is due to the fact that the highest density of states corresponds to the lower parts of the energy spectra which are less influenced by the self-consistency.

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