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

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Abstract. The effect of strong magnetic fields parallel to GaAs/Ga$_x$Al$_{1-x}$As interface on the subband structure of a 2D electron layer is investigated theoretically. The 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, there was suggested \[1\] that the deviations of the 2D Fermi line from the circular shape, which are due to 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 two-dimensional inversion layers at interfaces of GaAs/Al\(_x\)Ga\(_{1-x}\)As heterostructures.

Zawadzki, Klahn and Merkt \[2\] studied theoretically Fermi lines of narrow-band-gap semiconductors of the In-Sb type. Their analysis is based on two main simplifications: i) The confining potential \(V_{\text{conf}}(z)\) is taken in the form of a triangular potential well. ii) The interface is considered as an unpenetrable hard wall which is accounted for by an appropriate boundary condition for the wave function. 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 not too high magnetic fields and for this range of fields also the change of Fermi lines from the circular to the ‘egg-like’ form is expected.

In semiconductors with larger effective mass like GaAs the effect of parallel magnetic field should be less pronounced and, therefore, it was till now treated mainly by the perturbation theory \[3\]. On the other hand it is well known that due to the small conduction band offset between GaAs and Al\(_x\)Ga\(_{1-x}\)As the interface wall is rather soft and electrons can partly penetrate into Al\(_x\)Ga\(_{1-x}\)As. Thus, to obtain quantitatively better results, it is desirable to go beyond the triangular well approximation or the perturbation approach. For this reasons we decided to perform the full numerical self-consistent study of the influence of the in-plane magnetic field on the subband shape of 2D electron gas confined to GaAs/Al\(_x\)Ga\(_{1-x}\)As interface and this contribution presents its results.

It is now well-established that the numerical self-consistent calculation based on the effective mass approximation describes correctly the observed electron subband structure in the zero magnetic field. Moreover, generally accepted methods of such calculation including 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\textsubscript{x}Ga\textsubscript{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\textsubscript{x}Ga\textsubscript{1-x}As and ionized residual acceptors in GaAs:

$$\rho(z) = e \left[ N_e(z) - N_{d}^{+}(z) + N_{a}^{-}(z) \right].$$

(1)

We accept a 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 $-l_d - w \leq z \leq -w$ and $N_{a}^{-}(z) = N_a$ for $0 \leq z \leq l_a$, $w$ is the spacer thickness (see figure 1). The confining potential

$$V_{\text{conf}}(z) = V_0(z) + V_{s.c.}$$

(2)

is a sum of the step function $V_0(z) = V_0\Theta(-z)$ corresponding to the conduction band discontinuity and of the Hartree term $V_{s.c.}(z)$ determined from the Poisson equation

$$\frac{d^2 V_{s.c.}}{dz^2} = - \frac{\rho(z)}{\varepsilon}.$$  

(3)

The conduction band offset $V_0$ and the dielectric constant $\varepsilon$ enter our calculations as input parameters.

The simplest semiempirical model working quantitatively for the lowest conduction states of GaAs/Al\textsubscript{x}Ga\textsubscript{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\textsubscript{x}Ga\textsubscript{1-x}As are smoothly matched at the interface.

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

$$\psi_{\alpha}(\mathbf{r}) = \frac{1}{\sqrt{S}} e^{i(k_xx + k_yy)} \varphi_{i,k_x}(z)$$

(4)

and the Schrödinger equation may be written as

$$\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + \frac{1}{2m} \left( \hbar k_x - |e| B_y z \right)^2 - eV_{\text{conf}}(z) \right] \varphi_{i,k_x}(z) =$$

$$= \left[ E_i(k_x) - \frac{\hbar^2 k_y^2}{2m} \right] \varphi_{i,k_x}(z)$$

(5)
where the magnetic field parallel to the layer plane $x - y$ has a form $\mathbf{B} \equiv (0, B_y, 0)$. As the heterostructure is in an 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 the 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 $V_b = 300\text{meV}$ and the dielectric constant $\varepsilon = 12.9$.

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 $V_{\text{conf}}$ 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 continued by the full self-consistent calculation for $B \neq 0$ yielding the final results.

The parameters $N_d = 2 \times 10^{18}\text{cm}^{-3}$, $N_a = 10^{13}\text{cm}^{-3}$ and $w = 2\text{nm}$ were chosen to obtain the electron system of $N_e \approx 14 \times 10^{11}\text{cm}^{-2}$ having two levels occupied in zero magnetic field and depleting the second level at $\approx 10\text{T}$. 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 into the solution of coupled Poisson and Schrödinger equations.

In the zero magnetic field the in-plane electron motion and its out-of-plane component along the $z$-axis are completely independent. It means that all electrons within a subband are described by a single localized wavefunction $\varphi_i(z)$ regardless 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 $V_{\text{eff}}$ composed from the harmonic magnetic potential and the confining potential $V_{\text{conf}}$ is built

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

The centre $z_0$ of the magnetic part of the effective potential is related to the
wave vector component $k_x$ by $z_0 = \hbar k_x / m \omega$. Thus the magnetic field couples the electron motion in $x$ and $z$ directions and for each $k_x$ new $\varphi_{i,k_x}(z)$ 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 $\varphi_{i,k_x}(z)$ are shifted from their original positions $\langle z \rangle_0$ and $\langle z \rangle_1$ obtained for $B = 0$ and, therefore, also the charge distribution described by their squares is changed.

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

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

which makes it possible to calculate this quantity without numerical difficulties. As there is 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 $V_{\text{conf}}$. The dashed lines correspond to 'intermediate' results while the full lines describe the results of the full self-consistent calculations.

We already mentioned that in the zero magnetic field electrons reach all possible energies for just two centres of mass $\langle z \rangle_0$ and $\langle z \rangle_1$. If the 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 $\langle z \rangle_{i,k_x,\text{min}}$ and $\langle z \rangle_{i,k_x,\text{max}}$ 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

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

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

The difference between two types of calculations 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 $B = 12T$.

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

Individual wave functions are even more influenced by the magnetic field. Figure 4 shows the first subband wave functions $\varphi_{0,k_x}(z)$ 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 $Al_xGa_{1-x}As$ 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 a double-peak structure of the wave function for $B = 6T$.

We conclude that as in the case of the zero magnetic field the electron structure of GaAs/Al$_x$Ga$_{1-x}$As heterostructure 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 remain constant. It is due to the fact that the highest density of states corresponds to the bottom part of the energy spectra which are less influenced by the self-consistency.
References

[1] Leadley D R, Nicholas R J, Harris J J and Foxon C T 1990 20th International Conference on Physics of Semiconductors eds E M Anastassakis and J D Joannopoulos (Singapore: World Scientific Publishing Co.) p 1609

[2] Zawadzki W, Klahn S, Merkt U 1986 Phys. Rev. B33 6916

[3] Bastard G Wave mechanics applied to semiconductor heterostructures (Paris) p 317

[4] Stern F, Das Sarma S 1984 Phys. Rev. B30 840

[5] Ando T 1982 J. Phys. Soc. Japan 51 3893
Figure captions

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

Figure 2. Electron eigenenergies $E(z)$ calculated as a function of $\langle z \rangle_{i,k_z}$ and the confining potential $V(z)$. The energies are measured from the Fermi energy. Dashed lines correspond to the ‘intermediate’ results, full lines to the results of the full self-consistent calculations.

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

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