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In-plane magnetic-field-induced anisotropy of 2D Fermi contours and the field-dependent cyclotron mass

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Abstract. The electronic structure of a 2D gas subjected to a tilted magnetic field, with a strong component parallel to the GaAs/AlGaAs interface and a weak component oriented perpendicularly, is studied theoretically. It is shown that the parallel field component modifies the originally circular shape of a Fermi contour while the perpendicular component drives an electron by the Lorentz force along a Fermi line with a cyclotron frequency given by its shape. The corresponding cyclotron effective mass is calculated self-consistently for several concentrations of 2D carriers as a function of the in-plane magnetic field. The possibility of detecting its field-induced deviations from the zero-field value experimentally is discussed.

1. Introduction

The energy level structure of quasi-two-dimensional systems in magnetic fields tilted with respect to the sample plane have attracted attention for many years. As shown by Maan [1] and Merlin [2] the electron spectra can be found analytically for the special case of parabolic quantum wells. This simple analytically solvable model is very useful when discussing the qualitative aspects of 2D electron physics in quantum wells, but when the semiquantitative comparison of results with experimental data is the goal of investigation, more realistic models must be used and numerical methods of calculation employed.

The widely accepted approach to the electronic structure of realistic quantum wells in tilted magnetic fields, which relies on perturbation theory, was reviewed by Bastard [3]. It can be outlined as follows. The Hamiltonian is decomposed into three parts, $H = H_{\|} + H_{\perp} \bullet H_{\rm int}$. The first part $H_{\|}$ describes the motion of an electron in the z direction under the combined influence of the confining potential and the in-plane component of the magnetic field. If the in-plane field is not too strong its effect is usually included via perturbation theory. The second part of the Hamiltonian $H_{\perp}$ corresponds to the standard 2D gas subjected to the perpendicular component of the field and can be diagonalized analytically. In most situations the third coupling term $H_{\rm int}$ can be completely neglected or treated as a small perturbation. Only in certain special cases, for example when crossing of Landau levels from different subbands is important, the matrix elements of a coupling term must be evaluated and the Hamiltonian H diagonalized numerically [4].

In this paper we present a slightly different approach to the electron structure of quantum wells in tilted magnetic fields which is appropriate when the perpendicular component of the applied magnetic field is weak. Assuming for a moment $\boldsymbol{B} \equiv (0, B_y, 0)$, i.e. the field is exactly parallel to the plane of the 2D electron gas, the Hamiltonian $H_{\|}$ of an electron confined to the x–y plane by a potential $V_{\rm conf}(z)$ can be written as

$$H_{\|} = \frac{1}{2m}\left(p_x - eB_y z\right)^2 + \frac{1}{2m}p_y^2 + \frac{1}{2m}p_z^2 + V_{\rm conf}(z). \tag{1}$$

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Its energy spectrum is formed by subbands, momentum operators p_x and p_y commute with $H_\parallel$ and the eigenenergies $E_n(k_x, k_y), n = 0, 1, \ldots$ are functions of the quasi-continuous wavevectors k_x and k_y. The 2D Fermi surfaces, or more accurately the Fermi contours, are then defined separately for each subband by the equation $E_F = E_n(k_x, k_y)$.

The in-plane magnetic field B_y does not influence the electron motion in the y-direction while the electrons moving in the x-direction are decelerated or accelerated by the combined effect of the crossed fields B_y and $E_z = -\mathrm{d}V_{conf}(z)/\mathrm{d}z$, depending on the form of $V_{conf}(z)$. Consequently, it is expected that the subband separation, the 2D density of states and the shape of the Fermi contour will vary with increasing B_y [3]. Only recently have realistic self-consistent calculations of electron energy spectra in heterostructures subjected to parallel magnetic fields been performed [5, 6], enabling a quantitative estimate of these quantities.

Let the weak perpendicular component B_z of the magnetic field be added to the strong in-plane field component B_y. Then the electron dynamics in the x–y plane can be described semiclassically, in a similarly way to the dynamics of electrons in metals with non-spherical Fermi surfaces. The corresponding quasi-classical theory was originally developed by Onsager [7] and Lifshitz [8]; now it is a part of standard textbooks devoted to solid state physics (see, for example, [9]). According to this theory electrons move in the k space along trajectories defined by intersections of a Fermi surface and planes perpendicular to the applied magnetic field. In the 2D case there is only one such line, identical to the Fermi line itself. Once the k-space orbit is known, semiclassical theory predicts that the electron real space trajectory is of an identical shape except for the scale factor $\hbar/|e|B_z$, and rotation by $\pi/2$. The anisotropy of the Fermi contour due to the strong parallel field thus leads to the deviation of the electron trajectory from the originally circular form.

The modification of the Fermi contour shape by the in-plane magnetic field should manifest itself through the field dependence of the cyclotron effective mass m_c. This important characteristic of electron energy spectra is related to the Fermi area S_F surrounded by the Fermi contour by the semiclassical expression

$$m_c = \frac{\hbar^2}{2\pi}\frac{\mathrm{d}S_F}{\mathrm{d}E}. \tag{2}$$

Note that the field dependence of m_c is determined by the combined influence of the in-plane component of the magnetic field and of the shape of the confining potential $V_{conf}(z)$ of the quantum well and, therefore, the different structures with different quantum wells can be distinguished by measuring this quantity.

Two methods are widely used to determine the cyclotron effective mass of 2D electrons confined to the GaAs/AlGaAs interface: the cyclotron resonance in the infrared region of optical spectra [10] and the temperature damping of Shubnikov–de Haas oscillations [11]. To gain insight into the feasibility of such experiments, we report in this paper the results of self-consistent calculations of the field dependence of the cyclotron effective mass in the electron layer confined to the interface of the standard GaAs/AlGaAs heterostructure for several concentrations of 2D carriers.

2. Electronic structure in tilted magnetic fields

As mentioned above, non-interacting electrons mobile in the x–y plane and confined by the potential $V_{conf}(z)$ in the z direction are considered. A tilted magnetic field $\boldsymbol{B} = (0, B_y, B_z)$ is applied to the system. The corresponding one-electron Hamiltonian is

$$H = \frac{1}{2m}(\boldsymbol{p} - e\boldsymbol{A})^2 + V_{conf}(z) \tag{3}$$

where e and m are the electron charge and effective mass, respectively. We choose the vector potential $\boldsymbol{A}$ to be of the form $\boldsymbol{A} = (-B_z y + B_y z, 0, 0)$ which can be split into a sum $\boldsymbol{A} = \boldsymbol{A}_\perp + \boldsymbol{A}_\parallel$ of vector potentials $\boldsymbol{A}_\perp = (-B_z y, 0, 0)$ and $\boldsymbol{A}_\parallel = (B_y z, 0, 0)$ describing the perpendicular and parallel components of the magnetic field, respectively.

To bring the above Hamiltonian to a form similar to (1) we introduce new canonical momenta by

$$\begin{aligned} \pi_x &= p_x - eA_{\perp x} = p_x - m\omega_z y \\ \pi_y &= p_y - eA_{\perp y} = p_y \end{aligned} \tag{4}$$

where ω_z denotes $|e|B_z/m$. These momenta correspond to the in-plane electron motion, and the perpendicular component of the magnetic field B_z enters the Hamiltonian exclusively through them.

While quantum mechanics must be used to obtain the correct picture of electron motion in the z direction, both quantum mechanical and classical descriptions are acceptable for the in-plane motion when the perpendicular component of the magnetic field B_z is weak. The reason is that the weak perpendicular component yields many occupied Landau levels below the Fermi energy. The Landau levels near the Fermi energy are represented by states with high quantum numbers and, as is well known, they can be treated quasi-classically as well as quantum mechanically. Therefore, in the first step of our approximate description, the in-plane canonical variables and momenta (including the part $\boldsymbol{A}_\perp$ of the vector potential) will be considered as classical variables which commute with the Hamiltonian and enter it as c-numbers. Introducing further the components of the wavevector, k_x and k_y, by $\pi_x = \hbar k_x$ and $\pi_x = \hbar k_x$, respectively, we obtained a one-dimensional Hamiltonian identical to (1).

Again, the energy spectrum of this Hamiltonian is formed by subbands and the eigenenergies $E_n(k_x, k_y)$ are continuous functions of the wavevectors k_x and k_y or, equivalently, of the in-plane canonical momenta π_x and π_y. Since the perpendicular component of the magnetic field is hidden in the wavevector component k_x, the Hamiltonian describes the 2D system subjected only to the parallel field $\boldsymbol{B} = (0, B_y, 0)$. The shape of subbands is determined by both the confining potential and the in-plane magnetic field and can be accurately obtained by a self-consistent numerical calculation.

In the second step of our approximate treatment the single-subband effective Hamiltonian H_{eff} for the in-plane electron motion is constructed from a subband energy $E_n(k_x, k_y)$ by the backward substitution $k_x \to \pi_x/\hbar$, $k_y \to \pi_y/\hbar$. We get

$$H_{\text{eff}} = E_n(\pi_x, \pi_y) \tag{5}$$

and this effective Hamiltonian will be used to describe the electron motion in the x–y plane by standard Hamilton equations

$$\begin{aligned} \dot{x} &= \partial H_{\text{eff}}/\partial p_x \qquad \dot{y} = \partial H_{\text{eff}}/\partial p_y \\ \dot{p}_x &= -\partial H_{\text{eff}}/\partial x \qquad \dot{p}_y = -\partial H_{\text{eff}}/\partial y. \end{aligned}$$

The time derivatives of coordinates define the velocity components $v_x = \dot{x}$, $v_y = \dot{y}$ and yield the expressions

$$v_x = \frac{1}{\hbar}\frac{\partial E_n}{\partial k_x} \qquad v_y = \frac{1}{\hbar}\frac{\partial E_n}{\partial k_y}. \tag{6}$$

The time derivatives of momenta lead to

$$\hbar\dot{k_x} = -|e|B_z v_y \qquad \hbar\dot{k_y} = |e|B_z v_x. \tag{7}$$

These are the classical equations of motion for an electron subjected to the Lorentz force $e(v \times B)$, $B = (0, 0, B_z)$. Their solutions are in the form of orbits of all energies; among them, the orbit corresponding to the Fermi energy is the most important. A simple geometrical analysis allows us to derive the following properties of orbits.

As already mentioned, an electron is driven by the Lorentz force around the Fermi contour in the k plane. In the x–y plane, it executes an orbit similar in shape but scaled in dimensions by $\hbar/|e|B_z$ and turned through $\pi/2$. It has also a z component of motion which will be discussed later.

The period T of the cyclotron motion, or equivalently the cyclotron frequency ω_c, are obtained from (6) and (7) by direct integration. Since the magnitude of these parameters depends linearly on the amplitude of the perpendicular field component, it is more convenient to characterize the orbits by the cyclotron effective mass m_c defined with a help of the equation $\omega_c = |e|B_z/m_c$. The explicit expression relating m_c to the shape of the Fermi contour is

$$m_c = \frac{\hbar^2}{2\pi} \oint \frac{dk}{|\nabla_k E|} \tag{8}$$

where dk denotes an element of a length of the Fermi line. More often, the equivalent expression (2) is used.

It is well known that, unlike in the 3D case, the area S_F surrounded by the k-space orbit in 2D systems is identical to the Fermi area, which is determined by the concentration N_e of free carriers. Since the density of states g is related to the concentration by $g = dN_e/dE$ we can write

$$N_e = \frac{2}{(2\pi)^2} S_F \qquad g = \frac{2}{(2\pi)^2} \frac{dS_F}{dE} \tag{9}$$

where spin degeneracy is included. Making use of these expressions and of equation (2) a simple relation between the density of states and the cyclotron mass is obtained:

$$g = \frac{m_c}{\pi\hbar^2}. \tag{10}$$

Quantization of the in-plane electron motion by B_z can be taken into account using the Bohr–Sommerfeld quasi-classical quantization rules which state that each quantized real-space trajectory encloses an integer number of flux quanta $\hbar/|e|$. This procedure yields a discrete spectrum of Landau levels and the density of states becomes a series of delta functions separated by $\hbar\omega_c$. Note that the filling factor of each level is $2|e|B_z/h$, i.e. independent of the cyclotron mass and the same as in the case of an exactly perpendicular magnetic field.

To estimate the validity of our approximate treatment of the electron spectra we consider a model in which a 2D system is confined to the x–y plane by a harmonic potential $V_{conf}(z) = m\Omega^2 z^2/2$. In this special case the eigenenergies can be found in an analytic form both for in-plane and tilted magnetic fields [1]. Assuming first $B_z = 0$, as before, we can write

$$E_n(k_x, k_y) = \hbar\tilde{\omega}(n + \tfrac{1}{2}) + \frac{\hbar^2 k_x^2}{2\tilde{m}} + \frac{\hbar^2 k_y^2}{2m} \qquad n = 0, 1, \ldots \tag{11}$$

where $\widetilde{\omega} = (\omega_y^2 + \Omega^2)^{1/2}$, $\omega_y = |e|B_y/m$ and $\widetilde{m} = m\widetilde{\omega}^2/\Omega^2$.

The magnetic-field-induced anisotropy is described by the new effective mass $\widetilde{m}$ for the x component of the electron motion, which grows with B_y. The Fermi contour is distorted from a circular shape to an elliptical shape. The zero-field Fermi radius k_{0F} is determined by $E_{0F} = \hbar^2 k_{0F}^2/2m$ where E_{0F} is the zero-field Fermi energy. Taking into account the changes in the energy spectrum and the Fermi energy due to the in-plane magnetic field, the equation $E_F = E_n(k_x, k_y)$ for a determination of the Fermi contour can be rewritten in the form

$$k_{0F}^2 = \frac{\Omega}{\widetilde{\omega}} k_x^2 + \frac{\widetilde{\omega}}{\Omega} k_y^2. \tag{12}$$

From this equation the cyclotron effective mass can be evaluated using (8), and we get

$$m_c = \sqrt{m\widetilde{m}}. \tag{13}$$

The corresponding cyclotron frequency can be written as $\omega_c = \Omega\omega_z/\widetilde{\omega}$.

These approximate results should be compared with the exact solutions obtained for a parabolic quantum well subjected to tilted magnetic fields:

$$\omega_{1,2} = \tfrac{1}{2}\{[\omega_y^2 + (\omega_z + \Omega)^2]^{1/2} \mp [\omega_y^2 + (\omega_z - \Omega)^2]^{1/2}\}. \tag{14}$$

It is easy to show that the lowest-order expansion of these expressions with respect to ω_z yields exactly the results obtained by our approximate method:

$$\omega_1 \approx \frac{\Omega}{\widetilde{\omega}} \omega_z \qquad \omega_2 \approx \widetilde{\omega}. \tag{15}$$

Both exact and approximate solutions are shown in figure 1.

3. Self-consistent calculations

The standard semiempirical model working quantitatively for the lowest conduction states of GaAs/AlGaAs 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. Since the effect of the effective mass mismatch is completely neglected, and the envelope functions of GaAs and AlGaAs are smoothly matched at the interface, the Schrödinger equation has a form given by (1).

The confining potential

$$V_{conf}(z) = V_b(z) + V_{sc}(z) \tag{16}$$

is the sum of the step function $V_b(z) = V_b\theta(-z)$ corresponding to the conduction band discontinuity between AlGaAs and GaAs and of a term describing the interaction of an electron with ions and the electron–electron interaction. This term should be calculated self-consistently, and can be written as

$$V_{sc}(z) = V_H(z) + V_{xc}(z). \tag{17}$$

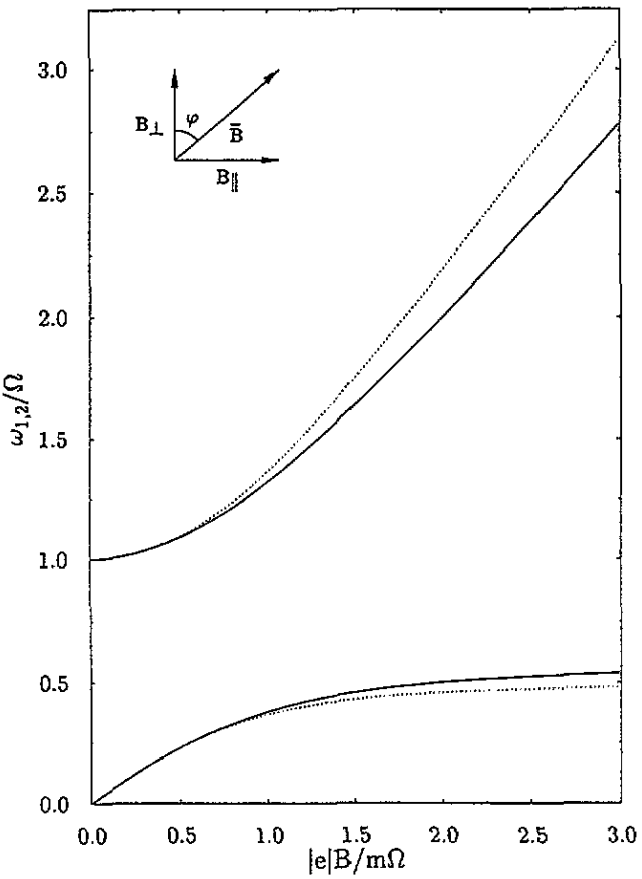

Figure 1. Eigenfrequencies of a parabolic quantum well subjected to a tilted magnetic field, $\varphi = 60°$. Dotted curves denote the exact solution, full curves the approximate one.

The Hartree term V_H is determined from the Poisson equation

$$\frac{d^2V_H}{dz^2} = \frac{|e|\varrho(z)}{\varepsilon} \tag{18}$$

and we use an expression calculated by Ruden and Döhler [12] in a density-functional formalism for the exchange correlation term V_{xc}:

$$V_{xc} \simeq -0.611\frac{e^2}{4\pi\varepsilon}\left(\frac{3N_e(z)}{4\pi}\right)^{1/3}. \tag{19}$$

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

For modulation-doped GaAs/AlGaAs heterostructures the total charge density $\varrho(z)$ in (18) can be split into parts corresponding to concentrations of electrons, $N_e(z)$, their parent donors in AlGaAs, $N_d^+(z)$, and ionized residual acceptors in GaAs, $N_a^-(z)$:

$$\varrho(z) = e[N_e(z) - N_d^+(z) + N_a^-(z)]. \tag{20}$$

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 $0 \leqslant z \leqslant l_a$, where w is the spacer layer thickness.

In our calculation, we consider a GaAs/AlGaAs heterostructure with parameters $N_d = 2 \times 10^{18}\,\mathrm{cm}^{-3}$, $N_a = 10^{14}\,\mathrm{cm}^{-3}$, the band offset $V_b = 225\,\mathrm{meV}$ and the dielectric constant $\varepsilon = 12.9$. Three selected values of the spacer layer thickness $w_1 = 40\,\mathrm{nm}$, $w_2 = 20\,\mathrm{nm}$ and $w_3 = 10\,\mathrm{nm}$ yield electron systems with three different concentrations of electrons: $N_{e1} \approx 1.8 \times 10^{11}\,\mathrm{cm}^{-2}$, $N_{e2} \approx 3.4 \times 10^{11}\,\mathrm{cm}^{-2}$ and $N_{e3} \approx 5.4 \times 10^{11}\,\mathrm{cm}^{-2}$, respectively. All these systems have only one occupied subband. The parameters l_a and l_d are determined in the course of the self-consistency procedure. For more details, see [6].

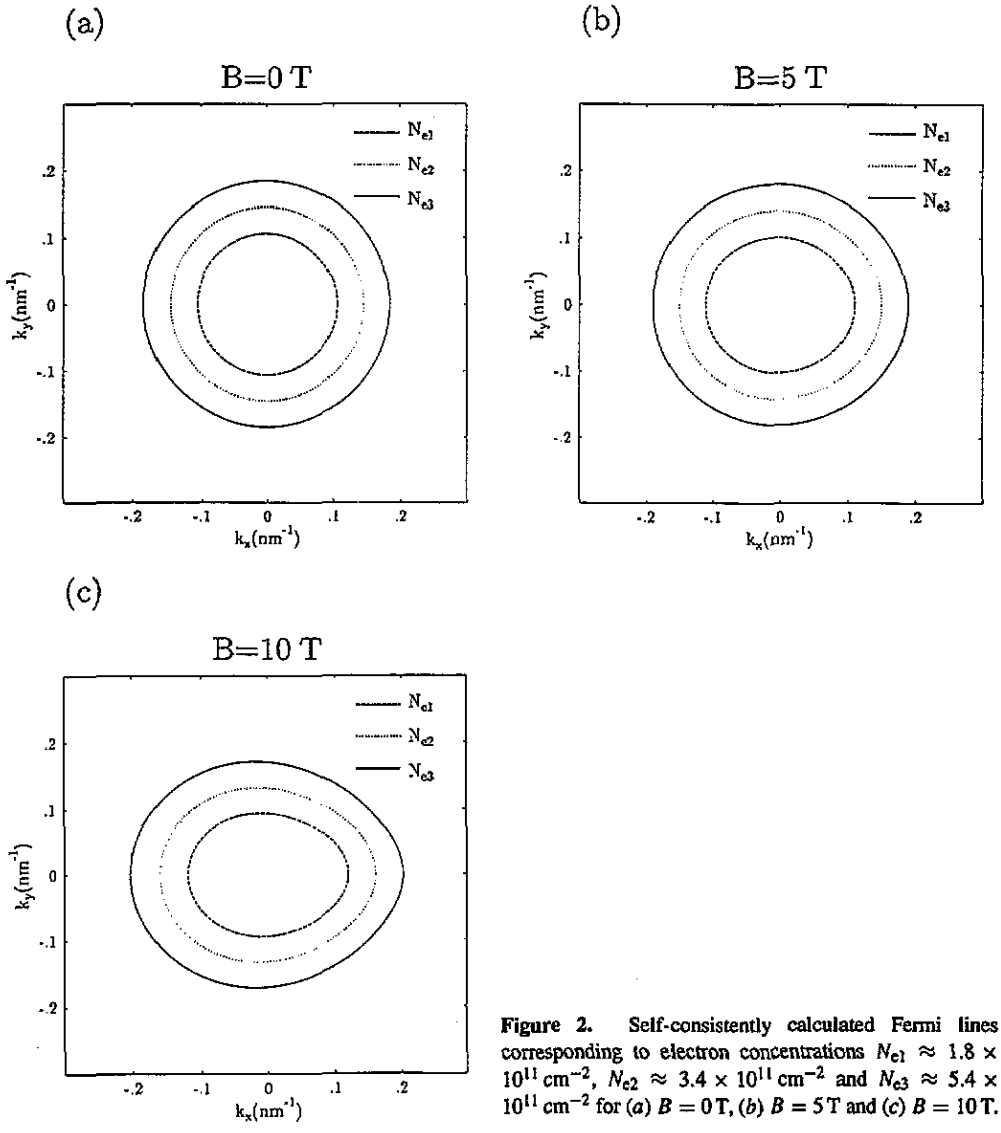

Figure 2. Self-consistently calculated Fermi lines corresponding to electron concentrations $N_{e1} \approx 1.8 \times 10^{11}\,\mathrm{cm}^{-2}$, $N_{e2} \approx 3.4 \times 10^{11}\,\mathrm{cm}^{-2}$ and $N_{e3} \approx 5.4 \times 10^{11}\,\mathrm{cm}^{-2}$ for (*a*) $B = 0\,\mathrm{T}$, (*b*) $B = 5\,\mathrm{T}$ and (*c*) $B = 10\,\mathrm{T}$.

The 'egg-like' Fermi contours calculated for the above three concentration and several magnitudes of the in-plane magnetic fields are shown in figure 2. The real-space trajectories

have similar shapes. Let us note that, since the average value of the out-of-plane coordinate of an electron $\langle z \rangle_{k_x}$ is a function of k_x, i.e. the position on the Fermi contour, the resulting trajectory does not lie exactly in the $x - y$ plane but is slightly tilted. It is elongated in the y direction and an electron is close to the interface at the wide end of the trajectory and in the bulk at its narrow end. A schematics of a classical real-space trajectory illustrating this behaviour is shown, together with its projection to the x–y plane, in figure 3.

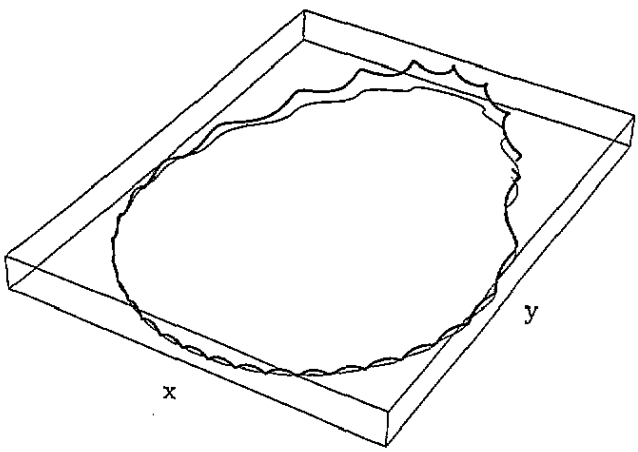

Figure 3. Schematics of a classical real-space trajectory of an electron in an electric and a tilted magnetic field (thick curve) and its projection onto the x–y plane (thin curve).

The field dependence of the cyclotron effective mass resulting from the self-consistent calculations is presented in figure 4. For all three electron concentrations the deviations of the cyclotron effective mass reach almost 25% of its zero-field value in a magnetic field $B_y = 10\,\mathrm{T}$.

4. Discussion and summary

The electronic structure of a 2D electron gas in GaAs/AlGaAs heterostructure subjected to a tilted magnetic field has been studied theoretically. We combine (i) self-consistent quantum mechanical calculations of the electron subbands of the 2D electron system in the presence of a parallel magnetic field and (ii) the subsequent quasi-classical description of the in-plane electron motion under the influence of the perpendicular magnetic field component.

The parallel magnetic field combined with the confining effect of the quantum well is the reason for deviations of the Fermi contour from a circular shape. Note that in this case the nature of the changes is different than in case of a standard modification of the Fermi line due to a periodic potential. Here, the time-reversal symmetry is broken by the magnetic field and, consequently, the Fermi contour has no inversion symmetry in k space, if the quantum well is asymmetric.

The quasi-classical quantization of the in-plane electron motion yields eigenenergies linear in the perpendicular component of the magnetic field. The method is applicable if the energy separation of subbands is larger than the separation of the Landau levels. It does not

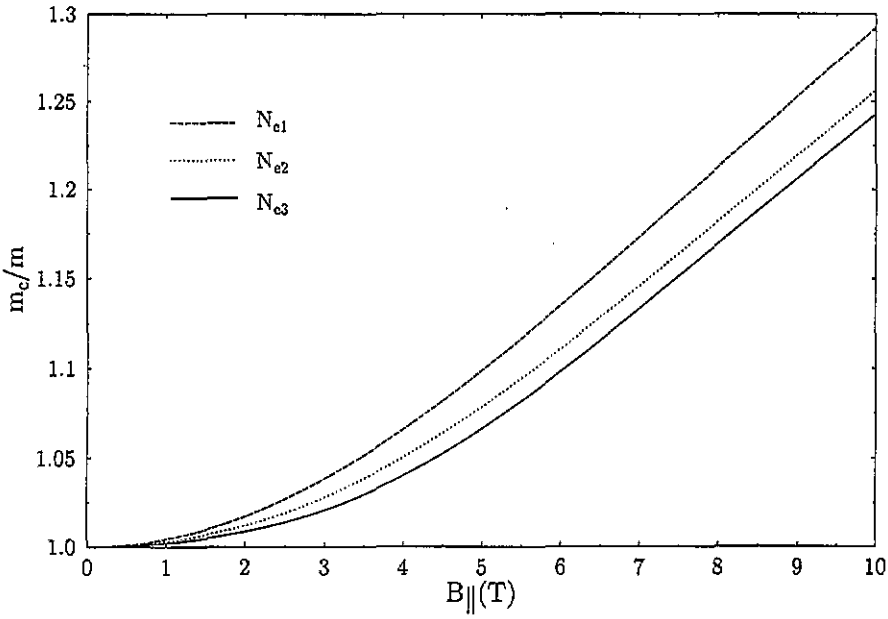

Figure 4. Self-consistently calculated in-plane magnetic-field dependence of the relative cyclotron mass corresponding to electron concentrations $N_{e1} \approx 1.8 \times 10^{11}\,cm^{-2}$, $N_{e2} \approx 3.4 \times 10^{11}\,cm^{-2}$ and $N_{e3} \approx 5.4 \times 10^{11}\,cm^{-2}$.

necessarily mean that the parallel magnetic field component must be always greater than the perpendicular one, but the in-plane field increases the subband separation.

The deviations of eigenenergies from a linear dependence for higher perpendicular magnetic fields are attributed to the fact that the real-space trajectories do not lie exactly in the x–y plane, as already mentioned in previous sections. In this case the quantization rules should not only take into account the perpendicular component of the magnetic field and the area surrounded by the projection of a trajectory to the x–y plane, but also the full field and the area of the trajectory itself.

The in-plane magnetic-field dependencies of the cyclotron mass were calculated in the limit of an infinitesimally small perpendicular component of the magnetic field. The changes in the cyclotron mass are surprisingly large and, to our knowledge, fully measurable by present experimental techniques.

Acknowledgments

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