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Electron g -Factor and Cyclotron Effective Mass in Semiconductor Quantum Wells Under Growth-Direction Applied Magnetic Fields

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The Ogg-McCombe effective Hamiltonian for the electron in the conduction band together with the non-parabolic and effective-mass approximations were used in a theoretical study of the cyclotron effective mass and electron effective Landé g_{\parallel} -factor in semiconductor GaAs-Ga_{1-x}Al_xAs quantum wells under an applied magnetic field parallel to the growth direction of the quantum well. Calculations are performed as a function of the applied magnetic field, and for different widths of the GaAs-Ga_{1-x}Al_xAs quantum wells. Results for the electron cyclotron effective mass and g_{\parallel} -factor are found in quite good agreement with experimental data.

Keywords: g -factor; Cyclotron effective mass; Quantum wells; Magnetic field

The understanding of the physics of semiconductor single and multiple quantum wells (QWs), quantum-well wires (QWWs), quantum dots (QDs), and superlattices (SLs) has been of great interest, and several studies have been performed to elucidate the physical properties of these systems [1–6]. The possible use of electron spins in the architecture of a solid-state based quantum computer has raised special attention in the study of the behavior of the electron spin coupled with an external magnetic field. In the single qubit operation it is of fundamental importance to have pure spin states in order to guarantee that no losses occur when the spins transport information [1]. This goal may be achieved by manipulating the electron g -factor in semiconductor heterostructures and designing appropriate external gate control devices. The cyclotron effective mass and electronic g -factor are of importance in possible applications and in the interpretation of experimental data in specific research fields such as magneto-optical and magneto-transport studies, optically detected nuclear-resonance experiments, spin electronics and quantum beats measurements, and in the fractional and integer quantum Hall effects [2–6].

The appropriate calculation of the electron g -factor and cyclotron effective mass depends on the detailed understanding of the interaction between the externally applied magnetic field and electronic states of the semiconductor heterostructure. Techniques such as electron spin resonance, Hanle effect, spin quantum beats, spin flip Raman scattering experiments, and capacitance and energy spectroscopies [4–10] have been used to measure the electron g -factor in semiconductor systems. Lattice effects on the orbital contribution, quantum-confinement, and application of hydrostatic-pressure and external electric/magnetic fields may considerably modify the conduction-electron g -factor, in both magnitude and sign, in different semiconductor heterostructures. On the other hand, experimental measurements of both the Landé g -factor and cyclotron effective mass provide an excellent tool for testing theoretical predictions of band-structure electronic calculations in low-dimensional semiconductor heterostructures. In

that respect, in this study we present a theoretical model which is used to give a proper physical and quantitative explanation of a series of experiments involving quantum beats and optically detected cyclotron resonance (ODCR) techniques applied in the measurements of g -factors and cyclotron effective masses of semiconductor GaAs-Ga_{1-x}Al_xAs QWs under growth-direction applied magnetic fields [2–5].

The Ogg-McCombe Hamiltonian, acting in the two-fold Γ_{6c} spin-degenerate conduction band of the bulk materials of the GaAs-Ga_{1-x}Al_xAs QW under an applied magnetic field parallel to the growth z -direction, is obtained within the effective-mass approximation and in fourth-order of \mathbf{k}, \mathbf{p} perturbation theory as [11–18]

$$\begin{aligned} \hat{H} = & \frac{\hbar^2}{2} \hat{\mathbf{K}} \frac{1}{m^*} \hat{\mathbf{K}} \hat{\mathbf{I}} + \frac{1}{2} g \mu_B B \hat{\sigma}_z + \Gamma \hat{\sigma} \cdot \hat{\mathbf{t}} + a_1 \hat{\mathbf{K}}^4 \hat{\mathbf{I}} + \frac{a_2}{l_B^4} \hat{\mathbf{I}} \\ & + a_3 [\{\hat{K}_x^2, \hat{K}_y^2\} + \{\hat{K}_x^2, \hat{K}_z^2\} + \{\hat{K}_y^2, \hat{K}_z^2\}] \hat{\mathbf{I}} \\ & + a_4 B \hat{\mathbf{K}}^2 \hat{\sigma}_z + a_5 \{\hat{\sigma} \cdot \hat{\mathbf{K}}, \hat{K}_z B \hat{\mathbf{I}}\} + a_6 B \hat{\sigma}_z \hat{K}_z^2 \\ & + V(z) \hat{\mathbf{I}}, \end{aligned} \quad (1)$$

where $\hat{\mathbf{I}}$ is the 2×2 unit matrix, $\hat{\mathbf{K}} = \hat{\mathbf{k}} + e\hat{\mathbf{A}}/\hbar c$, $\hat{\mathbf{k}} = -i\nabla$, and the Landau gauge is used for the vector potential $\mathbf{A} = -yB\hat{\mathbf{x}}$. The a_i , $i = 1 - 6$, are appropriate constants taken from Golubev *et al* [14] and with equal values for the well and barrier materials. $V(z)$ is the square-well confining barrier potential, taken as 60% of the Ga_{1-x}Al_xAs and GaAs band-gap offset [19], and m^* and g are the z growth-direction position-dependent conduction-electron effective mass and Landé g -factor, respectively [20]. The constant Γ is associated with the cubic Dresselhaus [21] spin-orbit term (due to the fact that GaAs has no inversion symmetry), $l_B = \sqrt{\frac{\hbar c}{eB}}$ is the Landau length, μ_B is the Bohr magneton, $\hat{\sigma} = (\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z)$, where the $\hat{\sigma}_i$ are the Pauli matrices, and $\hat{\mathbf{t}}$ is a vector operator with components given as $\hat{t}_x = \hat{K}_y \hat{K}_x \hat{K}_y - \hat{K}_z \hat{K}_x \hat{K}_z$ and corresponding cyclic permutations. The above Hamiltonian is a 2×2 conduction-band effective Hamiltonian [13–15], and includes

effects of non-parabolicity by taking into account the coupling between the lowest Γ_{6c} conduction band, Γ_{7v} and Γ_{8v} valence bands, and the Γ_{7c} and Γ_{8c} p-antibonding conduction bands. This Hamiltonian is expected to give a realistic description of the conduction-band Landau levels in zincblende-type semiconductors, semiconductor QWs, heterostructures, and so on. The second term in the RHS of (1) is the Zeeman contribution, the second-order in \mathbf{K} spin-dependent terms (with the factors a_4 , a_5 , and a_6) together with the third one (the spin-orbit Dresselhaus interaction), of third order in \mathbf{K} , contribute to changes in the heterostructure effective g -factor. The terms in a_1 and a_3 govern the energy dependence of the cyclotron effective mass, whereas the term with the factor a_2 gives the diamagnetic shift of the Landau electronic levels.

Note that k_x is a good quantum number (as \hat{H} does not explicitly depend on x) and the eigenfunctions of \hat{H} may be chosen as $\psi(\mathbf{r}) = \phi(y, z)e^{ik_x x}/\sqrt{L_x}$, where L_x is the QW length along the x direction and $\psi(\mathbf{r})$ and $\phi(y, z)$ are two-component wavefunctions. We now write the Hamiltonian as $\hat{H} = \hat{H}_0 + \hat{W}$, where \hat{W} may be neglected, as it may be shown to contribute only small corrections to the energy levels [22] (details of the calculation will be published elsewhere [23]). The eigenfunctions of \hat{H} (or \hat{H}_0) may then be written as

$$|+ \rangle = \psi_+(\mathbf{r}) = \frac{\exp(ik_x x)}{\sqrt{L_x}} \begin{pmatrix} \Phi_n(y)f_{n,m}^+(z) \\ 0 \end{pmatrix} \quad (2)$$

$$|- \rangle = \psi_-(\mathbf{r}) = \frac{\exp(ik_x x)}{\sqrt{L_x}} \begin{pmatrix} 0 \\ \Phi_n(y)f_{n,m}^-(z) \end{pmatrix} \quad (3)$$

where the \pm symbols correspond to \uparrow spin up or \downarrow spin down states, respectively, with the eigenfunctions $\Phi_n(y)$ of the one-dimensional (1D) harmonic oscillator [24] given by

$$\Phi_n(y) = \frac{1}{\sqrt{n! 2^n l_B \sqrt{\pi}}} e^{-\frac{(y-y_0)^2}{2l_B^2}} H_n\left(\frac{y-y_0}{l_B}\right), \quad (4)$$

where the H_n are the Hermite polynomials, $y_0 = k_x l_B^2$ is the orbit-center position, and $E_n = \hbar\omega_c(n + \frac{1}{2})$, with $n = 0, 1, 2, \dots$, and $w_c = \frac{eB}{m^*c}$, are the corresponding 1D energies. Notice that the subindex $m = 1, 2, 3, \dots$, in both $f_{n,m}^\pm(z)$ and the associated electronic levels $E_{n,m}^\pm$, indicates the m -th QW confined energy state, and $n = 0, 1, 2, \dots$, for a given m , represents the corresponding Landau subband energy levels [25]. The functions $f_{n,m}^\pm(z)$ and $E_{n,m}^\pm$ Landau energy levels may be obtained in a straightforward way [23] for a semiconductor GaAs-Ga_{1-x}Al_xAs QW. Of course, in the absence of the applied magnetic field, there are no Landau levels, the subband electronic states are only labelled by m , the problem reduces to that of confined electrons in a QW, and $E_{n,m}^\pm = E_m^\pm$, with m being the subband index of the energy levels in a GaAs-Ga_{1-x}Al_xAs QW.

In order to compare our theoretical results with available experimental measurements, we present calculations performed for GaAs-Ga_{0.65}Al_{0.35}As QWs. Figure 1 displays the

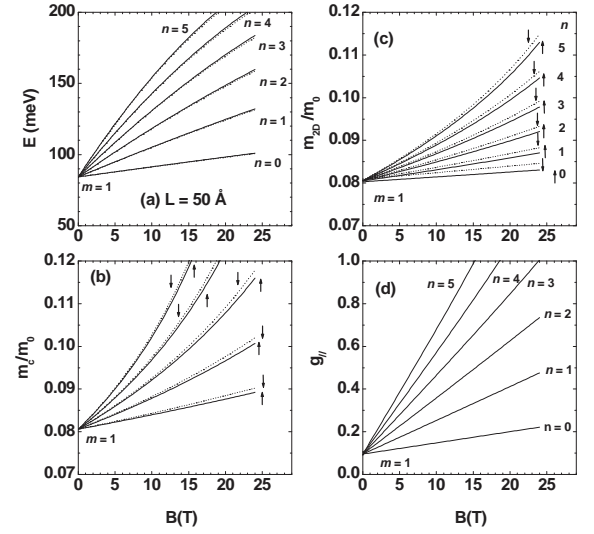


FIG. 1: (a) Electronic Landau levels, (b) $m_c^{\uparrow,\downarrow}$ cyclotron effective mass, (c) $m_{2D}^{\uparrow,\downarrow}$ 2D cyclotron effective mass, and (d) $g_{||}$ -factor, in an $L = 50$ Å GaAs-Ga_{0.65}Al_{0.35}As QW as functions of the growth-direction applied magnetic field. Full (dotted) lines correspond to spin up (\uparrow) (down \downarrow) electron Landau levels.

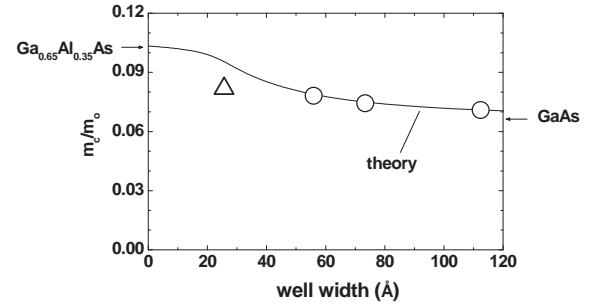


FIG. 2: Cyclotron effective mass for GaAs-Ga_{0.65}Al_{0.35}As QWs as a function of the well widths. Present theoretical results are given as a full curve, and experimental data are represented as an open triangle and open circles, from experimental measurements by Singleton *et al* [2] and Michels *et al* [3], respectively. The arrow at the left (right) vertical axis indicates the value of the m_c cyclotron effective mass corresponding to bulk Ga_{0.65}Al_{0.35}As (bulk GaAs).

magnetic-field dependence of the $E_{n,m}^\pm$ electronic Landau levels, the cyclotron effective mass

$$m_c^{\uparrow,\downarrow} = (\hbar e B / c) / [E_{n+1}^{\uparrow,\downarrow}(B) - E_n^{\uparrow,\downarrow}(B)], \quad (5)$$

the two-dimensional (2D) cyclotron effective mass

$$m_{2D}^{\uparrow,\downarrow} = (\hbar e B / c) (n + 1/2) / [E_n^{\uparrow,\downarrow}(B) - E_n^{\uparrow,\downarrow}(B = 0)], \quad (6)$$

and parallel g factor,

$$g_{||} = [E_n^{\uparrow}(B) - E_n^{\downarrow}(B)] / (\mu_B B), \quad (7)$$

for an $L = 50$ Å GaAs-Ga_{0.65}Al_{0.35}As QW. The definition of the $m_c^{\uparrow,\downarrow}$ cyclotron effective mass is convenient for com-

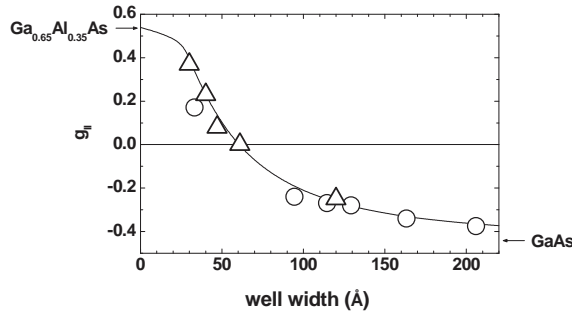


FIG. 3: $g_{||}$ -factor for GaAs-Ga_{0.65}Al_{0.35}As QWs as a function of the well widths. Present theoretical results are given as a full curve, and experimental data are represented as open triangles and circles, from experimental measurements by Le Jeune *et al* [4] and Malinowski *et al* [5], respectively. The arrow at the left (right) vertical axis indicates the value of the $g_{||}$ -factor corresponding to bulk Ga_{0.65}Al_{0.35}As (bulk GaAs).

parison with experimental measurements involving transitions between consecutive Landau levels, whereas the $m_{2D}^{\uparrow,\downarrow}$ 2D cyclotron effective mass is appropriate for experiments associated with, for instance, resonant magnetotunneling in double barrier heterostructures [26]. Results shown in Figure 1 correspond to calculations associated to the electronic levels of the first $m = 1$ subband of Landau states. The nonlinear behavior of the $E_{n,m=1}^{\pm}$ Landau electronic levels in Fig. 1(a) is due to the presence of non-parabolic terms in the Hamiltonian, and it is apparent that the effects of nonlinearity are stronger for the highest Landau levels and large values of the applied magnetic field, as compared with the effects on the lowest Landau states. The above mentioned properties of the Landau energy levels lead to the behavior of the cyclotron masses as shown in Figs. 1(b) and 1(c), which evolve from an essentially linear function of the applied magnetic field, for the lowest levels and small values of B , to a strong nonlinear behavior as a function of B , for the highest Landau levels and large values of the applied field. The field-dependence of the $g_{||}$ -factor [cf. Fig. 1(d)] is due both to the magnetic-field effect on the electronic Landau levels as well as to the confinement/barrier penetration of the electron envelope wave function due to the presence of the Ga_{0.65}Al_{0.35}As barriers. Although not shown here, for large values of the QW width, e.g., $L \gtrsim 200$ Å, the influence of the barriers on the Landau levels is negligible as compared to that of the magnetic field, the electronic envelope wave functions essentially do not penetrate in the Ga_{0.65}Al_{0.35}As barriers, and the $g_{||}$ field dependence, for $n = 0$, on the QW width is small. Calculated results for the m_c cyclotron effective mass as a function of the width of the GaAs-Ga_{0.65}Al_{0.35}As QW are

depicted in Fig. 2 and compared with experimental results by Singleton *et al* [2] and Michels *et al* [3]. Theoretical results are for small values of the applied magnetic field ($B \approx 0$), and for the $m = 1, n = 0$ Landau level. As one may see from Fig. 2, the agreement with experimental data by Michels *et al* [3] is excellent, and we find a fair only agreement with the open triangle value by Singleton *et al* [2]. Figure 3 shows the present theoretical results for the $g_{||}$ -factor, in the case of the $m = 1, n = 0$ Landau level, as a function of the GaAs-Ga_{0.65}Al_{0.35}As QW width. Again, calculated results are for small values of the growth-direction applied magnetic field ($B \approx 0 - 4$ T), and are compared with the experimental data by Le Jeune *et al* [4] (for B in the range from 1 T to 4 T), and Malinowski *et al* [5] (for $B = 4$ T). Notice that, for large QW widths, the value of the $g_{||}$ -factor approaches the $g = -0.44$ value of bulk GaAs, as expected. Also, it is apparent in Fig. 3 that the present theoretical calculations are in excellent agreement with the experimental measurements.

Summing up, we have used the effective-mass approximation and taken into account the non-parabolic-band effects via the Ogg-McCombe effective Hamiltonian, to theoretically evaluate the electronic Landau levels, cyclotron effective masses and $g_{||}$ -factors of GaAs-Ga_{1-x}Al_xAs semiconductor QWs. The characteristic problem of the Ogg-McCombe Hamiltonian is solved by expressing the corresponding spin \uparrow and \downarrow envelope wave functions as products of harmonic-oscillator and QW wave functions. We have obtained the $m_c^{\uparrow,\downarrow}$ cyclotron effective mass, the $m_{2D}^{\uparrow,\downarrow}$ and the $g_{||}$ -factor as functions of the QW widths and growth-direction applied magnetic fields, with the calculated results exhibiting a noticeable dependence on the strength of the applied magnetic field. Finally, present theoretical calculations for the Landé cyclotron effective mass and $g_{||}$ -factor in isolated GaAs-(Ga,Al)As QWs were found in quite good agreement with the experimental measurements reported by Singleton *et al* [2], Michels *et al* [3], Le Jeune *et al* [4] and Malinowski *et al* [5].

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