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How the size quantisation is destroyed in a one-dimensional wire under a strong longitudinal magnetic field

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Abstract. The electronic states in a cylindrical quantum well (CQW) in the presence of a strong axial magnetic field are investigated numerically. We have found that the size quantisations due to the lateral confinements may be destroyed by the strong magnetic field and, when the applied field is larger than a critical magnetic field, the quantised energy levels associated with the radial quantum numbers ($n = 2, 3, 4, \ldots$) are completely smeared out, except the first radial quantised energy level associated with $n = 1$. The numerical calculation predicts a critical magnetic field $B_c \propto R^{-2}$, where R is the radius of the CQW. Using the results obtained, we have successfully explained an unexpected experimental phenomenon related to the damping of oscillations of the density of states in a quasi-one-dimensional wire under a strong longitudinal magnetic field.

For nearly a decade, studies of the quantum Hall effect (QHE) in a two-dimensional (2D) system in the presence of a strong magnetic field perpendicular to the 2D layer have attracted much interest. The Landau quantisation induced by the transverse magnetic field plays a very important role in the QHE, but the effect of the longitudinal magnetic field parallel to the 2D layer is somewhat subtle. Several papers [1] have dealt with the effect of the longitudinal magnetic field on the collective modes. However, in a quasi-one-dimensional (quasi-1D) quantum well wire the motion of electrons is quantum mechanically confined in two directions. In this case, a longitudinal magnetic field will play an essential role owing to the mixing of electronic and magnetic quantisation.

Recently, it was observed [2] that a new anisotropy exists in a quasi-1D electron system in the presence of a magnetic field. The density of states changes dramatically when a magnetic field is applied along different axes of the sample. In particular, it was found that an appropriate magnetic field (in the x direction) parallel to the wires may completely destroy the electric quantisation related to the lateral confinements, which is an intriguing and unexpected phenomenon which has not yet been understood.

When the longitudinal magnetic field is applied, two lateral confinements as well as the magnetic confinement are strongly mixed. The electrons remain free in the longitudinal direction (essentially 1D). It is evident that for a 1D wire with rectangular cross section, when the ratio of the two lateral sizes is too small (or too large), the confinement in one direction becomes much stronger than that in the other direction, and then these two lateral confinements may decouple each other. If the cross section is chosen to be a circle, on the other hand, coupling between lateral confinements will be the strongest. Here we present a simple model calculation to explain this fact qualitatively.

For simplicity, we consider an electron gas confined in an infinite cylindrical quantum well (CQW) with a radius R in the presence of a magnetic field B_0 along the axial direction; then we can directly write the effective-mass Hamiltonian describing an electron in the CQW [1] using the symmetric gauge:

$$H = -(\hbar/2\mu^*)[\partial^2/\partial z^2 + \partial^2/\partial r^2 + (1/r)\partial/\partial r + (1/r^2)\partial^2/\partial\varphi^2] - (\mathrm{i}e\hbar B_0/2\mu^* c)\partial/\partial\varphi + (e^2B_0^2/8\mu^* c^2)r^2 + V_{\mathrm{eff}}(r). \tag{1}$$

Here, (r, φ, z) are the cylindrical coordinates, and the effective radial potential $V_{\mathrm{eff}}(r) = 0$ for $r < R$ and $V_{\mathrm{eff}}(r) = \infty$ for $r > R$. The electronic wavefunction can be written as [1]

$$|n, m, k\rangle = \exp[\mathrm{i}(kz + m\varphi)]\, F_{n,m}(r) \tag{2}$$

where $F_{n,m}(r)$ is the eigenfunction for motion in the radial effective potential $V_{\mathrm{eff}}(r)$, m is the angular quantum number, k is the wavevector along the axial direction and n is the radial quantum number relating to the numbers of nodes of the wavefunctions. Substituting equations (1) and (2) into the Schrödinger equation gives the following radial equation:

$$[r^2\,\mathrm{d}^2/\mathrm{d}r^2 + r\,\mathrm{d}/\mathrm{d}r - (m^2 - \varepsilon_{n,m}r^2 + r^4/4a_{\mathrm{L}}^4)]\, F_{n,m}(r) = 0 \tag{3}$$

where

$$\omega_{\mathrm{c}} = eB_0/\mu^* c \qquad a_{\mathrm{L}} = (\hbar c/eB_0)^{1/2}$$
$$\varepsilon_{n,m} = (2\mu^*/\hbar)(E_{n,m} - \hbar^2k^2/2\mu^* - m\hbar\omega_{\mathrm{c}}/2). \tag{4}$$

ω_{c} is the cyclotron frequency and a_{L} is the Landau radius (magnetic length). Introducing two dimensionless quantities

$$x = \varepsilon_{n,m}^{1/2}r \qquad \beta_{n,m} = 1/2a_{\mathrm{L}}^2\varepsilon_{n,m} \tag{5}$$

where $\beta_{n,m} \propto (R/a_{\mathrm{L}})^2$ if n, m are given, we obtain the solution of equation (3):

$$F_{n,m}(x) = Lh_m[(x_n^{(m)}/R)r] = \sum_{j=0}^{+\infty} a_{m+2j}\left(\frac{x_n^{(m)}r}{R}\right)^{m+2j} \tag{6}$$

with the recurrence relation of the coefficients

$$a_{m+2j} = (\beta_{n,m}^2 a_{m+2j-4} - a_{m+2j-2})/4j(m+j) \tag{7}$$

and

$$a_m = 1/2^m m! \qquad a_{m+2} = -1/2^{m+2}(m+1)! \tag{8}$$

Here $x_n^{(m)}$ stands for the nth node of the function $Lh_m(x)$. The energy levels are given by

$$E_{n,m} = \hbar^2k^2/2\mu^* + \hbar^2(x_n^{(m)})^2/2\mu^* R^2 + m\hbar\omega_{\mathrm{c}}/2. \tag{9}$$

In particular, when $\beta_{n,m} = 0$ (or $B_0 = 0$), $Lh_m(x)$ will reduce exactly to the mth-order Bessel function $J_m(x)$. The wavefunctions $Lh_0(x)$ and $Lh_1(x)$ for different values of $\beta_{n,m}$

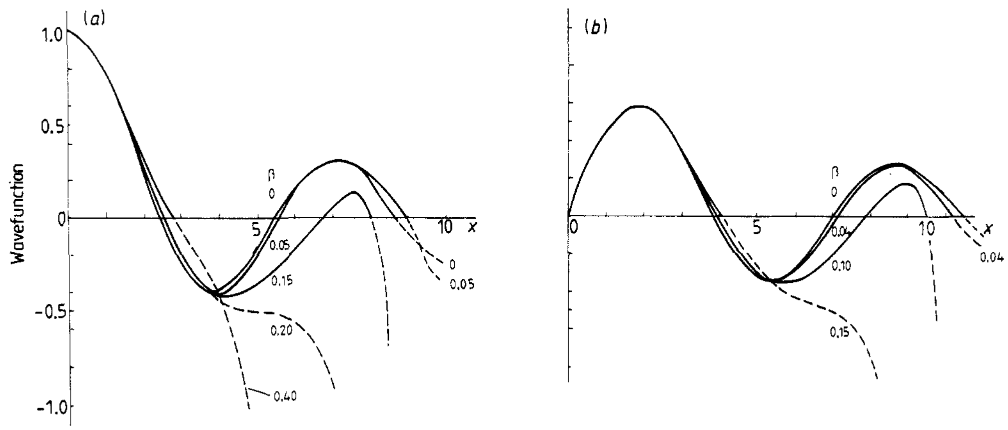

Figure 1. The wavefunctions (*a*) $Lh_0(x)$ and (*b*) $Lh_1(x)$ for different values of $\beta_{n,m}$. From it we can see how the nodes gradually degenerate two by two.

are shown in figure 1. Here the magnetic field B_0 is a single valued and monotonically increasing function of $\beta_{n,m}$. For given $\beta_{n,m}$, the $\beta_{n,m}$ dependence of the magnetic field B_0 changes with different states or different values of n and m. From this we know that the nodes of $Lh_0(x)$ and $Lh_1(x)$ will gradually degenerate two by two with increasing $\beta_{n,m}$ (or B_0), except that finally only the first node remains. Above a critical value $\beta^c_{1,m}$, all the nodes, except the first node, will disappear. Of course, $\beta^c_{1,m}$ changes with different angular quantum numbers m, which implies that only the electronic state with radial quantum number $n = 1$ exists for any given value of m in this case. It should be noted that $\beta_{n,m}[x_n^{(m)}]^2 = \Phi/\Phi_0 = g_{n,m}$ is the quantum flux, which is a physical quantity independent of the radius R of the CQW, although the critical magnetic field B_c may depend on it. From equation (9) we also know that the nodes $x_n^{(m)}$ are related to the radial quantisation of energy for different m. Figure 2 presents the magnetic field dependence of energy levels for $R = 750$ Å, $\mu^* = 0.041m_e(Al_{1-x}Ga_xAs\text{–}GaAs)$ and $k = 0$. Here the free motion of electrons along the axial direction is not affected by the magnetic field, and it decouples with the radial and azimuthal motion of electrons; then we can choose $k = 0$ for simplicity. From figure 2 we can see the evident diamagnetic shifts of the energy levels. It should be noted that the meanings of 'radial excited state' and 'radial ground state' below are different from the general meanings of the excited and ground states. They are just introduced to sign the states for simplicity. If the magnetic field is strong enough, all the excited states with radial quantum number $n =$ 2, 3, 4, . . . for any given value of angular quantum number m, which are referred to the 'radial excited state' here, will degenerate two by two and then disappear on further increase in B_0. Here we show only the degeneration of energy levels of $E_{0,2}$ and $E_{0,3}$. Also, if $B_0 > 4.450$ T (or $\beta_{n,m} > 0.40$), we see that the energy level $E_{1,1}$ of the first 'radial ground state' will be approximately proportional to the magnetic field B_0. This implies that the electrons have nearly been localised at the boundary of CQW, which is usually called the edge state [3–5]. Here the states with radial quantum number $n = 1$ are referred to as the 'radial ground states'. When $n = 1$ and $m = 1, 2, 3, \ldots$, these are first, second, third, . . . 'radial ground states', respectively. However, $n = 1$ and $m = 0$ represent the real ground state of the system. When $B_0 = 0.589$–3.604 T, the energy $E_{1,1}$

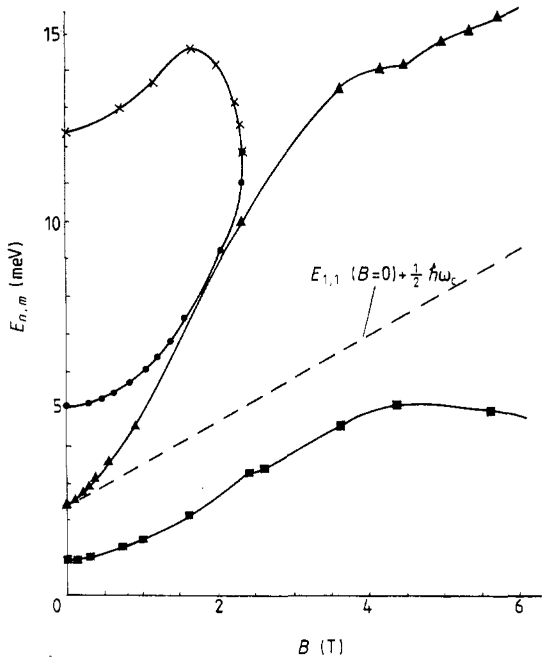

Figure 2. The magnetic field dependence of energy levels $E_{n,m}$ for different values of the quantum numbers: ■, $n = 1$, $m = 0$; ▲, $n = 1, m = 1$; ●, $m = 0, n = 2$; ×, $m = 0$, $n = 3$. The parameters are given by $R = 750$ Å, $\mu^* = 0.041\ m_e$ and $K = 0$.

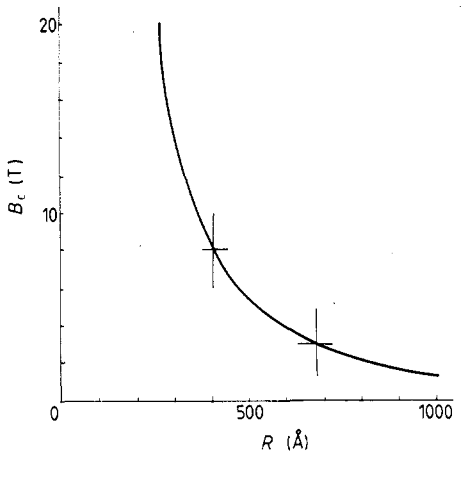

Figure 3. The dependence of the critical magnetic field on radius R. The curve shows the relation $B_c \propto R^{-2}$.

of the first 'radial ground state' increases dramatically and then deviates greatly from the decoupling behaviour (in which $E_{1,1} = E_{1,1}$ $(B_0 = 0) + \hbar\omega_c/2)$.

Numerical calculation shows that the critical quantum flux $g^c_{1,m} = \beta^c_{1,m}[x_1(m)]^2$ satisfies $g^c_{1,0} > g^c_{1,1} > \ldots > g^c_{1,m} > \ldots$, e.g., $g^c_{1,0} = 8.86$, and $g^c_{1,1} = 8.50$. It can easily be seen that, for given m, $x_2(m)$ and $x_3(m)$ are the last pair of nodes to degenerate, e.g., the nodes $x_2(0)$ and $x_3(0)$ for $m = 0$ as shown in figure 1. Using the maximum of $g^c_{1,m}$, the critical magnetic field can be estimated as

$$B_c = (\Phi_0/\pi R^2)g^c_{1,0} \tag{10}$$

which is shown in figure 3, in which $B_c \propto R^{-2}$ is an important theoretical prediction. This is rather obvious on dimensional grounds: the crossover from 3D to 1D behaviour must occur at some critical value of the dimensionless parameter $\Lambda = R/a_L$, i.e., $\Lambda_c = eB_cR^2/hc$ or $B_c \propto R^2$.

Indeed, although the geometric structures used are different, we can still compare qualitatively the theoretical result obtained with the experimental result given by figure 3 of [2]. In [2], two lateral sizes L_y and L_z of the quasi-1D wire with rectangular cross section are about 100 Å and 3000 Å, respectively. When the longitudinal magnetic field B_0 is about 8.0 T, the oscillation of the density of states, which arises because of the changes in the Fermi energy and occurs when the Fermi energy crosses a 1D sub-band (in the CQW model these 1D sub-bands are referred to as the energy levels $E_{n,0}$ of 'radial excited states' for $n = 2, 3, 4, \ldots$ and $m = 0$), completely disappears. We think that, when the magnetic field $B_0 > B_c$, only the energy levels $E_{1,m}$ of the 'radial ground states' are retained, but $\hbar\omega \simeq 22.6$ meV is so large that we cannot see the $E_{1,m}$ ($m = 1, 2, 3, \ldots$) energy levels in figure 3 of [2]. In principle, the magnetic levels in figure 3 of [2] corresponding to the $E_{1,m}$ ($m \geqslant 1$) energy levels in our model would be observed when the gate voltage is large enough to provide a higher electron density. As discussed above, we know that the damping of the 'radial excited states' ($n = 2, 3, 4, \ldots$), which is related to the damping of oscillations of the density of states in figure 3 of [2], is definite if the magnetic field is strong. Because the magnetic flux should remain the same in two different structures, we can estimate the effective radius R_{eff} of the CQW with a geometrical structure factor $\gamma \geqslant 1$:

$$R_{\text{eff}} = \gamma(L_yL_z/\pi)^{1/2}. \tag{11}$$

From figure 3, we estimate R_{eff} to be approximately equal to 382 Å for $B_c \simeq 8.0$ T.

If the magnetic field is applied along the direction perpendicular to the plane containing the quasi-1D wires, as shown in figure 1(a) of [2], the magnetic field couples the free motion (in the x direction) with the y-direction-confined motion. Thus, R_{eff} is relatively large ($a_L \simeq 148$ Å for $B_0 = 3.0$ T) compared with the case in which B_0 is along the longitudinal direction and, when $B_c \simeq 3.0$ T, we see the damping of oscillations of the 1D sub-bands except that the magnetic levels in figure 1(a) of [2] corresponding to the $E_{1,m}$ energy levels in the CQW are retained. In figure 2 of [2], the magnetic field couples the free motion (in the x direction) with the z-direction-confined motion. Because $L_z \simeq L_y/30$, R_{eff} is very small in this case compared with the case in which B_0 is along the direction perpendicular to the plane containing the quasi-1D wires; thus we do not see the damping of oscillations with B_0 up to 20 T, because of the very large critical magnetic field $B_c \simeq 90.0$ T given by equation (10) in this case. If the lateral size L_z is increased, e.g., $L_z = 500$ Å, we predict that the damping oscillations of the density of states as in figure 1(a) of [2] can be observed with B_0 above 18.0 T.

It should be pointed out that, although the comparison given here between the theoretical and the experimental result is not exactly quantitative, the relation between the critical magnetic field B_c and the radius of the CQW is an important theoretical prediction. We shall be carrying out experiments with different lateral sizes so as to verify the prediction $B_c \propto R^{-2}$ given by this theory.

Acknowledgments

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Appendix

In equation (5), we have introduced the parameter $\beta_{n,m}$ as

$$\beta_{n,m} = 1/2a_L^2\varepsilon_{n,m} = R^2/2a_L^2[x_n^{(m)}]^2 \tag{A1}$$

where $x_n^{(m)}$ is the nth node of the function $Lh_m(x)$. Furthermore, we have emphasised that the magnetic field B_0 should be a single-valued and monotonically increasing function of $\beta_{n,m}$, and the $\beta_{n,m}$ dependence of B_0 changes with different values of n and m. In fact, when B_0 is large enough, the magnetic length will be small compared with the radius R, and the system is essentially two dimensional. In such a case, $\beta_{n,m} \rightarrow \infty$ as $B_0 \rightarrow \infty$, and the transformation given by equation (5) is no longer effective, since the series in equation (6) does not converge as $\beta_{n,m} \rightarrow \infty$. Alternatively, we introduce another transformation in equation (6):

$$\xi = x^2/2a_L^2\varepsilon_{n,m} \tag{A2}$$

then equation (6) can be rewritten as

$$F_{n,m}(\xi) = A\exp(-\xi/2)\,\xi^{m/2}\,{}_1F_1[-(\varepsilon_{n,m}\hbar/2\omega_c\mu^* - m/2 - \tfrac{1}{2}), m+1, \xi] \tag{A3}$$

where A is a normalisation factor, ${}_1F_1(a, b, \xi)$ is the Kummer function and $\varepsilon_{n,m}$ satisfies the condition

$${}_1F_1[-(\varepsilon_{n,m}\hbar/2\omega_c\mu^* - m/2 - \tfrac{1}{2}), m+1, R^2/2a_L^2] = 0. \tag{A4}$$

It is clear that, in the region $0 < B_0 < \infty$, both equation (6) and equation (A4) give exactly the same result. When $B_0 \rightarrow \infty$, or $a_L \rightarrow 0$, in order to ensure that $F_{n,m}(\xi)$ is finite in the whole region $r \leqslant R$, the following condition must be satisfied:

$$\varepsilon_{n,m}\hbar/2\omega_c\mu^* - m/2 - \tfrac{1}{2} = n_r \tag{A5}$$

where n_r is a non-negative integer. Equation (A5) can be rewritten as [6]

$$E_{n,m} = \hbar\omega_c[n_r - (|m| - m)/2 + \tfrac{1}{2}] + \hbar^2k^2/2\mu^*. \tag{A6}$$

The quantum number n_r is just the Landau level index for positive values of m, while for negative values the Landau level index reads $n_r - |m|$. To be sure that $E_{n,m}$ must be positive, we know that $n_r = 0, 1, 2, 3, \ldots$, and $|m| \leqslant n_r$. It should be noted that the result in equation (A6) is an exact solution of equation (A4) only at the point $B_0 \rightarrow \infty$. In fact, equation (A4) is just a formal solution; it can only be solved in the way similar to that of equation (6). However, equation (A3) cannot give a reasonable result in another well known limiting case when $B_0 \rightarrow 0$, since the transformation in equation (A2) becomes trivial which gives $\xi \rightarrow 0$ as $B_0 \rightarrow 0$. On the contrary, equation (6) is able to give explicitly the exact solution as $B_0 \rightarrow 0$:

$$F_{n,m}(x) = J_m(x) \tag{A7}$$

where $J_m(x)$ is the mth order Bessel function.

From the discussion above, we know that equations (6) and (A4) give two different solutions for two well known limiting cases, i.e. $B_0 \rightarrow 0$ and $B_0 \rightarrow \infty$, respectively. Moreover, equations (6) and (A4) will give the same solution in the region $0 < B_0 < \infty$.

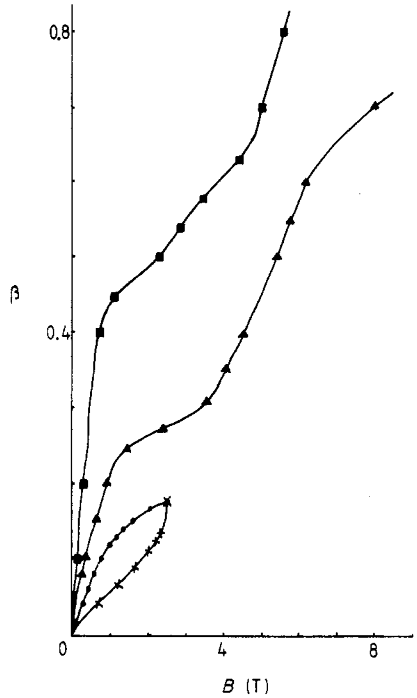

Figure A1. The dependence of the parameter $\beta_{n,m}$ on magnetic field B_0 for different values of the quantum numbers: ■, $n = 1$, $m = 0$; ▲, $n = 1$, $m = 1$; ●, $m = 0$, $n = 2$; ×, $m = 0$, $n = 3$. The radius is given by $R = 750$ Å.

Figure 4 presents the magnetic field B_0 dependence of the parameter $\beta_{n,m}$, and from this we can see that the magnetic field B_0 is a single-valued and monotonically increasing function of $\beta_{n,m}$. Equation (6) is valid for $0 \leqslant B_0 < \infty$, excluding the point $B_0 = \infty$, while equation (A4) is valid for $0 < B_0 \leqslant \infty$, excluding the point $B_0 = 0$. It is impossible to obtain the solution of equation (A4) at the point $B_0 = \infty$ from equation (6).

On the other hand, we should emphasise that the radial quantum number n and the Landau level index n_r or $n_r - |m|$ are totally different; they refer to the radial electric quantisation and the Landau quantisation, respectively, and the Landau quantisation only exists in a 2D system or in the high-field limit $B_0 = \infty$.

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