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Landau level broadening and thermodynamics in a two-dimensional electron system with a space charge distribution

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Abstract. We discuss space charge effects on Landau level broadening and various thermodynamic properties of a two-dimensional electron system in a magnetic field. In particular, the Landau level width is expressed in terms of the magnetic field and the space charge density. There exists a large diamagnetic spike in the magnetic moment when the cyclotron frequency becomes smaller than the harmonic-oscillator frequency introduced by the space charge distribution.

Recently Harrison [1] has discussed some novel effects of space charge and crossed electric fields on energy levels and low-temperature diamagnetism in two-dimensional electron gas (2DEG) systems. A quadratic electrostatic potential may arise from a uniform three-dimensional distribution of ionised donor impurities in a semiconductor [1–2]. The energy spectrum of the system has been shown to be quite different from the case without this space charge distribution [1]. The de Haas-van Alphen oscillations in low-temperature diamagnetism disappear when the space charge density is sufficiently large [1].

Besides Harrison's work, there exists a large body of studies on the so-called ultranarrow or *quasi-one-dimensional* electron devices (see e.g. [3–9]). A quadratic confining potential was also employed [7–9] to study various width or boundary effects in such systems. In contrast with these works, here we are concerned with only *two-dimensional* systems.

In the present paper the thermodynamics of a 2DEG in the presence of a space charge distribution is studied systematically. We shall first find the density of states, i.e., the Landau level broadening, of the system, from which the magnetic moment and the specific heat are calculated in a straightforward fashion.

Consider a 2DEG confined in the xy plane, in the presence of a uniform magnetic field B in the z-direction. Let there be a uniform three-dimensional space charge density ρ in the region $-L_y/2 \le y \le L_y/2$. We shall begin with a derivation of the electrostatic potential introduced by ρ . Suppose that the extension of the system in x direction is considerably larger than that in the y direction and yet the system is large enough to be considered two-dimensional. Thus the electric field due to the space charge distribution has only a component in the y direction and depends solely on y, because of the symmetry. By the same token, the electric field, E_y say, vanishes at y = 0. Consider an infinitesimal cylinder with its central axis along the y axis, located at (0, y, 0). Suppose the length and the radius of the cylinder are dy and r, respectively. By using Gauss's law on this cylinder, we find

$$[E_{y}(y + dy) - E_{y}(y)]\pi r^{2} = \pi r^{2} dy \rho/\varepsilon, \qquad (1)$$

where ε is the dielectric constant of the material and SI unit is used in this paper. Solving (1) for E_y and recalling $E_y(y=0) = 0$, we obtain $E_y(v) = (\rho/\varepsilon)v$, which corresponds to an electrostatic potential $\psi(y) = -(\rho/2\varepsilon)y^2$. For an electron with charge -e, the potential energy is

$$V(y) = (e\rho/2\varepsilon)y^2.$$
 (2)

We wish to comment that in the case where $L_x \sim L_y$, one may use a cylindrically symmetric potential, i.e., $V = (e\rho/2\varepsilon) (x^2 + y^2)$.

The Schrödinger equation with the Landau gauge A = (-By, 0, 0) and the potential given by (2) has been solved exactly by Harrison [1, 2]. The energy levels are

$$E_{n,k} = (n + \frac{1}{2})\hbar\omega + (\hbar^2 k^2 / 2m)(\gamma/\omega)^2$$
(3)

where n = 0, 1, 2, ...

$$\omega = (\omega_c^2 + \gamma^2)^{1/2} \tag{4}$$

 $\omega_{\rm c} = eB/m$ is the cyclotron frequency, and

$$\gamma^2 = \rho e / \varepsilon m. \tag{5}$$

In the following discussions we always assume that $\omega^2 = \omega_c^2 + \gamma^2 > 0$, otherwise the system will not be stable. The corresponding wave functions are [1, 2]

$$\varphi_{n,k}(x,y) = \left(e^{ikx} / (L_x)^{1/2} \right) U_n(y-Y)$$
(6)

where $U_n(r)$ is the *n*th simple harmonic oscillator eigenfunction centred at r = 0. The orbit centre here in (6) is (see footnote)

$$Y = \hbar k \omega_{\rm c} / \omega^2 m. \tag{7}$$

By imposing periodic boundary conditions $\varphi_n(x + L_x, y) = \varphi_n(x, y)$, one obtains

$$k = \pm 2\pi s / L_x$$
 $s = 0, 1, 2, \dots$ (8)

Following Landau [10], we determine the range of k values, as well as that of s in (8) by requiring that the orbit centre lies within the 2DEG region. In other words, we require that $-L_v/2 \le Y \le L_v/2$, or

$$k_{\min} \equiv -\omega^2 m L_y / 2\hbar\omega_c \le k \le \omega^2 m L_y / 2\hbar\omega_c \equiv k_{\max}.$$
 (9)

We note that this restriction can be regarded only as an approximation since a zero potential [10], as well as a quadratic potential in the present case, is inconsistent with such a restriction. This approximation may be valid only if the system is fairly large so that detailed perimeter effects can be neglected.

[†] In [1], the space charge region is chosen to be $0 \le y \le L_y$. Because of the symmetry, the electrostatic potential should be $2\pi\rho(y - L_{y/2})^2$ in cgs units, instead of $2\pi\rho y^2$ given by equation (1) of [1]. This difference, however, only shifts the centre of electron orbits and does not influence the physical properties of the system, e.g. the energy levels.

From (8) and (9) we obtain the range of s, i.e. $s_{\min} \le s \le s_{\max}$, where

$$s_{\max} = \frac{k_{\max}L_x}{2\pi} = \omega^2 m(L_x L_y)/4\pi\hbar\omega_c = -s_{\min}.$$
 (10)

Hence the number of distinct states for each quantum number n is [1]

$$D = s_{\rm max} - s_{\rm min} = \omega^2 m A / 2\pi \hbar \omega_{\rm c} \tag{11}$$

where $A = L_x L_y$ is the 2D area. As argued above, it is not appropriate to use this result in a quasi-one-dimensional (or ultra-narrow) system.

In the following we shall derive the density of states from the above known results.

One notices that in the absence of the space charge, the energy levels given by (3) reduce to the Landau levels and are independent of k. Also, D reduces to the degeneracy of each Landau level. If one still wishes to consider the first term in (3), which is $(n + \frac{1}{2})\hbar\omega$, the Landau levels in the case of a non-zero density of space charge ρ , one finds that they are all shifted upward (downward) if $\rho > 0$ ($\rho < 0$). The k-dependent term in (3) may represent broadenings of Landau levels. These broadenings are therefore entirely asymmetric with respect to Landau level centres $(n + \frac{1}{2})\hbar\omega$, n = 0, 1, 2, ...

We rewrite the total density of states D(E) as a sum of the density of states associated with each broadened Landau level [11]:

$$D(E) = \sum_{n=0}^{\infty} \frac{D}{\Gamma} R_n \left(\frac{E - E_n}{\Gamma_n} \right) \equiv \sum_{n=0}^{\infty} D_n(E)$$
(12)

where $E_n = (n + \frac{1}{2})\hbar\omega$ and the level width Γ_n will be determined below. From (8), the number of states available between k and k + dk is $ds = (L_x/2\pi) dk$. Also, each energy state is two-fold degenerate, since $E_{n,k} = E_{n,-k}$. Hence

$$D_n(E) dE = 2 ds = 2(L_x/2\pi) dk \qquad k > 0.$$
 (13)

We solve (3) for k in terms of E and substitute into (13), yielding

where the level width is independent of the Landau level index:

$$\Gamma_n = (\hbar^2 k_{\max}^2 / 2m)(\gamma/\omega)^2 = m\omega^2 \gamma^2 L_y^2 / 8\omega_c^2 \equiv \Gamma.$$
(15)

Therefore the broadening shape function defined in (12) is

$$R_n(x) \equiv R(x) = \frac{1}{2}x^{-1/2} \qquad \text{for } 0 \le x \le 1$$

= 0 \qquad otherwise. (16)

It is transparent that $\int_0^{+\infty} dE D_n(E) = D$, or $\int_0^{+\infty} dx R(x) = 1$.

Now we discuss some interesting features revealed by the level width derived. We obtain from (5) that the characteristic energy associated with space charge density $\rho \equiv N_{sc}e$ is

$$\hbar\gamma \,\mathrm{meV} = 18.75 \,(N_{\rm sc}/2 \times 10^{17} \,\mathrm{cm}^{-3})^{1/2} (0.0665 \,m_0/m)^{1/2} \,(12/\varepsilon_{\rm r})^{1/2} \tag{17}$$

where ε_r is the relative dielectric constant. Harrison [1] used $N_{sc} = N_D$, where N_D is the donor density in the bulk material. Typically [12], $N_D = 2 \times 10^{17}$ cm⁻³. As we shall show, this assumption is plausible only in a quasi-one-dimensional sample.

In GaAs heterostructures, $m = 0.0665 m_0$, $\varepsilon_r = 12$, $\hbar\gamma$ is then considerably larger than the magnetic energy $\hbar\omega_c$, which is 8.7 meV for B = 5 Tesla.

The level width given by (15) can be rewritten as

$$\Gamma = \Gamma_0 [1 + (\hbar \gamma / \hbar \omega_c)^2]$$
⁽¹⁸⁾

where the square bracket contains the magnetic field dependence, and

$$\Gamma_0 = m\gamma^2 L_y^2 / 8 = L_y^2 N_{\rm sc} e^2 / 8\varepsilon_0 \varepsilon_{\rm r}$$

= 3.77 × 10¹² (N_{sc}/2 × 10¹⁷ cm⁻³)(12/\varepsilon_{\rm r})(L_y/1 cm)² (meV). (19)

Even for the smallest 2DEG samples, i.e., $L_y = 200 \ \mu m$, we find that $\Gamma_0 = 1.5 \times 10^9 \text{ meV}$ if $N_{sc} = N_D = 2 \times 10^{17} \text{ cm}^{-3}$ and $\varepsilon_r = 12$. Substituting it into (18), we learn that $\Gamma = 8.5 \times 10^9 \text{ meV} \ge \hbar \omega_c = 8.7 \text{ meV}$. Since the Landau levels are broadened so much, we expect that the number of occupied Landau levels will be very large. One can estimate a lower limit as follows. The Fermi level is $E_F \simeq n_F \hbar \omega_c$, where n_F is the index of the highest occupied Landau level. The fraction of total number of states under the Fermi level in the *i*th Landau band is $[(E_F - E_i)/\Gamma]^{1/2} \le (n_F \hbar \omega_c/\Gamma_0)^{1/2}$. Suppose the density of electrons and the magnetic field are such that in the absence of the space charge distribution, only the lowest Landau level is occupied (the strong magnetic field limit). Then $n_F [n_F(\hbar \omega_c/\Gamma_0)]^{1/2} \simeq 1$. In other words, $n_F \ge 10^3$, and $E_F \sim n_F \hbar \omega_c \ge 10^4 \text{ meV}$. This is obviously not true for an ordinary 2DEG system. Therefore it is possible for the space charge density to be close to the donor density only in a quasi-one-dimensional system.

An explanation for this is that most of the charged ions in the bulk material are heavily screened. Those screened charges only affect a small portion of electrons that are close to them. Hence they do not contribute to the long range y^2 potential shown in (2). One expects that the effective space charge density will be much lower than that of the donor, i.e., $N_{sc} \ll N_D$. But the question of how to estimate N_{sc} has, to our knowledge, not yet been answered. We hope that the following discussion on space charge effects on the thermodynamics of the system will shed some light on this matter.

For simplicity we assume that the Landau levels do not overlap, i.e.

$$\Gamma \leq \hbar\omega. \tag{20}$$

We shall also assume positive space charge distribution ($\rho > 0$). Hence the density of states is as shown in figure 1. At zero temperature, the free energy is equal to the total internal energy:

$$U = \int_{0}^{E_{\rm F}} ED(E) \, \mathrm{d}E$$

= $(D/2\Gamma^{1/2}) \{\frac{2}{3}n_{\rm F}\Gamma^{3/2} + n_{\rm F}^{2}\Gamma^{1/2}(\hbar\omega) + \frac{2}{3}[E_{\rm F} - (n_{\rm F} + \frac{1}{2})\hbar\omega]^{3/2}$
+ $2(n_{\rm F} + \frac{1}{2})\hbar\omega[E_{\rm F} - (n_{\rm F} + \frac{1}{2})\hbar\omega]^{1/2}\}$ (21)

where $E_{\rm F}$ is the Fermi energy, and we recall that $n_{\rm F}$ is the index of the highest filled





Figure 2. Magnetic moment for $\Gamma_0/\hbar_{\gamma} = 0.001$ and $2\pi\hbar n/m\gamma = 20$.

Landau level, i.e., $0 < E_F - (n_F + \frac{1}{2})\hbar\omega \leq \Gamma$. The Fermi energy can be determined from the total number of electrons N:

$$\int_{0}^{E_{\rm F}} D(E) \,\mathrm{d}E = N \tag{22}$$

or

$$E_{\rm F} = (n_{\rm F} + \frac{1}{2})\hbar\omega + (N/D - n_{\rm F})^2\Gamma$$
(23)

and

$$n_{\rm F} = [N/D] \tag{24}$$

where [x] is the largest integer that does not exceed x. Substituting (23) into (21), we obtain the total energy of the system:

$$U = \frac{1}{3}n_{\rm F}D\Gamma + \frac{1}{2}Dn_{\rm F}^2(\hbar\omega) + \frac{1}{3}D(N/D - n_{\rm F})^3\Gamma + (n_{\rm F} + \frac{1}{2})\hbar\omega(N - n_{\rm F}D).$$
(25)

It is also of interest to write down the average energy per electron u = U/N in terms of the filling factor

$$\nu = N/D = (2\pi\hbar n/m\gamma)(\omega_{\rm c}/\gamma)(1 + \omega_{\rm c}^2/\gamma^2)^{-1}.$$
(26)

$$u = \left[\frac{1}{2}n_{\rm F}^2\nu^{-1}(\hbar\omega) + (n_{\rm F} + \frac{1}{2})(1 - n_{\rm F}\nu^{-1})(\hbar\omega)\right] + \left[\frac{1}{3}n_{\rm F}\nu^{-1}\Gamma + \frac{1}{3}\nu^2(1 - n_{\rm F}\nu^{-1})^3\Gamma\right].$$
(27)



Figure 3. Specific heat for $kT/\hbar\gamma = 0.1$, $\Gamma_0/\hbar\gamma = 0.001$ and $2\pi\hbar n/m\gamma = 20$.

Now we are ready to evaluate the magnetic susceptibility. Since the internal energy u depends on the magnetic field B through ν , ω and Γ , taking the derivative with respect to B is quite lengthy, but straightforward. The result is

$$M/N = - \partial u/\partial B = -(2\mu_{\rm B})\{\frac{1}{3}n_{\rm F}\nu^{-1}(\Gamma/\hbar\omega_{\rm c})(1-4d) + \frac{1}{2}n_{\rm F}^{2}\nu^{-1}a^{1/2}(2-3d) + \frac{1}{3}\nu^{2}(\Gamma/\hbar\omega_{\rm c})[-2(1-n_{\rm F}\nu^{-1})^{3} + 2d(1-n_{\rm F}\nu^{-1})^{3} - 3(1-n_{\rm F}\nu^{-1})^{2}n_{\rm F}\nu^{-1}(1-2d)] - (n_{\rm F} + \frac{1}{2})n_{\rm F}\nu^{-1}a^{1/2}(1-2d) + (n_{\rm F} + \frac{1}{2})(1-n_{\rm F}\nu^{-1})a^{1/2}(1-d)\}$$
(28)

where

$$a = (1 + \gamma^2 / \omega_c^2)$$
 and $d = \gamma^2 / (\omega_c^2 a).$ (29)

It is easy to check that (27) and (29) reduce to their corresponding quantities of an ideal 2DEG [13] by letting $\Gamma = 0$.

At low temperatures, $\Gamma \gg kT$, so the specific heat can be calculated in a standard fashion [13]:

$$C_{v} = \frac{1}{3}\pi^{2}k^{2}TD(E_{\rm F})$$

= $(\frac{1}{3}\pi^{2}k^{2}T)D/2\Gamma^{1/2}1/[E_{\rm F} - (n_{\rm F} + \frac{1}{2})\hbar\omega]^{1/2}.$ (30)

Substituting (23) into (30), we obtain the average specific heat per electron:

$$C_{\nu}(Nk) = (\frac{1}{6}\pi^2) (kT/\hbar\gamma) (\Gamma/\hbar\gamma)^{-1} \nu^{-1} (\nu - n_{\rm F})^{-1}.$$
(31)

The magnetic moment and the specific heat plotted in figures (2) and (3) exhibit some interesting features. In particular, one sees that there is a large diamagnetic spike in the region where $\omega_c/\gamma \leq 1$. Also, the specific heat peaks change 'parity' at $\omega_c/\gamma = 1$, where a δ -peak exists. This feature can be qualitatively explained from (31) as follows. $C_v/(Nk)$ shows a spike (singularity) each time the filling factor ν reaches an integer, i.e., $\nu = n_{\rm F}$. From (26), we know that ν reaches its minimum at $\omega_c/\gamma = 1$ and increases monotonously as ω_c/γ increases or decreases from unity. This is the reason that the oscillations in $C_v/(Nk)$ should be somewhat symmetric with respect to $\omega_c/\gamma = 1$. Similarly one can show that the δ -peak at $\omega_c/\gamma = 1$ may be shifted if $(2\pi\hbar n)/(m\gamma)$ is not exactly an even integer as chosen in figure 3. As a first approximation, impurity scattering effects [14, 15] are not taken into account in the above discussions. When one considers these effects, Landau levels will be further broadened. One can argue that since the level broadening introduced by space charge is asymmetric with respect to the level centre and the broadening introduced by scatterings is symmetric [14, 15] the resultant level broadening should be asymmetric with respect to the level centre. The asymmetric broadening recently observed in experiment [16] can therefore be explained schematically by the above argument. It implies that the effects predicted in the present paper may possibly be significant and observable in these materials used in [16]. One may also expect that, as a result of impurity scatterings, the diamagnetic spike and asymmetric pikes in the specific heat will be further damped.

In summary, we have discussed the Landau level broadening and the thermodynamics of a 2DEG in the presence of a uniform magnetic field and a three-dimensional space charge distribution. In particular, we have derived an expression of the Landau level width in terms of the magnetic field and the space charge density. The Fermi energy, the magnetic moment and the specific heat have been calculated explicitly. We found a large diamagnetic spike in the magnetic moment when the cyclotron frequency becomes smaller than the harmonic oscillator frequency introduced by the space charge.

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