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Possibility for direct experimental determination of two-dimensional electron density of states

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The de Haas-van Alphen effect in strong magnetic fields in a two-dimensional electron system allows the direct determination of its density of states.

The nature of the density of states (DOS) in a strong magnetic field B is very relevant to the electronic properties of a two-dimensional electron system (2DES), in particular, for the quantized Hall effect. The latter, according to von Klitzing,¹ suggests a weak constant DOS "background" between Landau levels. A natural way to determine the DOS at the Fermi level is from measurements of a thermodynamic quantity, such as the magnetization or heat capacity.² (Another measure of the density of states is the inversion layer capacitance.³) de Haas-van Alphen (dHvA) measurements⁴ indicate, even in high-mobility single-quantum wells, a substantial DOS between Landau levels (in agreement with heat-capacity measurements²) when compared to theoretical calculations. The latter were performed for Gaussian Landau levels with the half-width $\Gamma \propto B^{1/2}$. Such Γ is consistent with short-range scatterers.⁵ However, the calculated amplitude is about four times smaller than experimental results.⁴ These authors conclude⁴ that there is no existing theoretical explanation for the DOS they observe. By virtue of the great importance of such a conclusion, one should eliminate an a priori assumption of Gaussian Landau levels.

It seems almost obvious that this may be done. Any thermodynanmic quantity A is related, in the end, only to the DOS $D(\epsilon)$. Therefore, the dependence of A(B) on magnetic field B should, in principle, allow one to determine the dependence of $D(\epsilon)$ on energy ϵ .

Explicitly, thermodynamic properties depend both on $D(\epsilon)$ and on the Fermi energy ϵ_F . The Fermi energy is itself related to $D(\epsilon)$ and B by the equation for the number of particles. Furthermore, $D(\epsilon)$ depends on ϵ and B via the Schrödinger equation (in a magnetic field) with an impurity potential. As a result, the relation between A(B) and $D(\epsilon)$ reduces in a general case to extraordinarily complicated functional equations. No wonder that no attempts were made to solve this problem without specific assumptions about $D(\epsilon)$ (e.g., its Gaussian form). To find an explicit solution, which would be unique, stable, and accurate, probably seemed hopeless. However, this is exactly what is done in this paper: I present an algorithm for a direct "mapping" of the magnetic susceptibility $\chi(B)$ on $D(\epsilon)$. This becomes possible due to several observations.

When scatterers are long ranged (compared to the magnetic length), the center of the Fermi-energy quantum cyclotron orbit moves along an equipotential line, $U = U_0$, and DOS reduces to the magnetic-field-independent area inside this line. This eliminates the task of solving the Schrödinger equation, but still reduces the problem to two functional equations. However, in magnetic fields where only the lowest Landau level (more specifically, the Landau subband) is occupied, one obtains the DOS together with other valuable information. Then I demonstrate that

$$U_0(B) - U' = \int_B^\infty (M_1 + \mu^*) dB$$
 ,

where $M_1(B) \equiv M/N$ is the magnetic moment per electron, N is the total number of electrons, U' is the minimal value of the impurity potential in a system, and μ^* is the Bohr magneton. Thus, U_0 is the area in the plot $M_1 = M_1(B)$.

The Fermi energy $\epsilon_F(B)$ and the DOS D(B) equal $\epsilon_F(B) = U_0 + \frac{1}{2}\hbar \Omega$; $D(B) = -N^2/B\chi$, where $\chi_1 \equiv \chi/N$ is the magnetic susceptibility per particle; Ω is the cyclotron frequency. These equations map $D(\epsilon_F)/N$ onto the plot of $1/B\chi_1$ against the renormalized area in $M_1 = M_1(B)$. Finally, the area $S(U_0)$ inside $U = U_0$ is provided by the plot of

$$S(B) = chN/2eB$$

against $U_0 = U_0(B)$. Thus, one directly (and obviously uniquely) determined DOS $D(\epsilon)$, the Fermi energy $\epsilon_F(B)$, and $S(U_0)$ in the interval of magnetic fields where only the lowest Landau level is occupied. In weaker magnetic fields, where the next Landau level appears, $D(\epsilon_F)$ may be determined in the next interval of ϵ_F , and so on. When DOS is determined in the whole (finite) range of potential energies in the system, then $M_1(B)$ can be calculated (with no adjustable parameters) in weaker fields and compared to the experimental $M_1(B)$. This allows one to determine the accuracy of the approach and the region of its validity. The calculations are done for the Landau diamagnetism when the number of particles N is preserved. However, they are readily generalized to, e.g., the calculation of heat capacity when N is not conserved. The real limitation to the whole approach is a one-particle DOS, i.e., relatively weak electron-electron interaction.

Now put these considerations into explicit formulas. Consider sufficiently strong magnetic fields (unfortunately either somewhat stronger than in Ref. 4 or applied to samples with lower electron density). When scatterers are long ranged compared to the magnetic length $l_0 = (c\hbar/eB)^{1/2}$, the center of a quantum cyclotron orbit moves along an equipotential line⁶ U = const, and an electron energy ϵ at the *j*th Landau level is $\epsilon \approx (j + \frac{1}{2})\hbar \Omega + U$, where $\Omega = eB/m^*c$ is the cyclotron frequency. (The small spin splitting is ignored.)

The area per flux quanta is hc/eB. Suppose S(U) is the total area inside all potential lines U; then the area change $\Delta S = (\partial S/\partial U) \Delta U$ yields $2\Delta S/(hc/eB)$ states, where 2 accounts for the spin degeneracy. The corresponding DOS

(per unit U) D(U),

$$D(U) = (2eB/ch)(\partial S/\partial U) , \qquad (1)$$

is the same for all Landau subbands. The Fermi energy $\epsilon_F = \epsilon_F(B)$ yields DOS (per unit ϵ)

$$D(\epsilon_F) = \sum_j D(U_j); \qquad (2)$$

$$U_j(B) = \epsilon_F(B) - (j + \frac{1}{2})\hbar \Omega \quad . \tag{3}$$

The summation is related to all $U' \le U_j \le U''$, where U' is a minimal and U'' is a maximal value of U, both of which are finite in a finite sample. Naturally, S(U) has its minimum S(U') = 0 and its maximum S(U'') = S, where Sis the total area of a sample. When $U \simeq U'$, then

$$S(U) \simeq \frac{1}{2} a (U - U')^2$$
 (3a)

In the approximation of Eqs. (1)-(3), two functions, S(U)and $\epsilon_F(B)$, determine all thermodynamic quantities, e.g., the magnetic moment M(B). In principle, if the total number of electrons N is preserved, N(B) = N(0) determines $\epsilon_F(B)$ via S(U). Then M(B) depends only on S(U) and determines it. This is the idea and the goal of the paper. In fact, $S(U_j) = S[\epsilon_F(B) - (j + \frac{1}{2})\hbar\Omega]$ is an unknown function of an unknown function $\epsilon_F(B)$. In general, two functional equations for $\epsilon_F(B)$ and S(U) are hardly solvable. But a strong magnetic field B leads to an easy solution. Just for simplicity, consider zero temperature and no inelastic scattering.

In strong magnetic fields $B > B^*$, when only the first Landau subband is occupied, DOS D(U) in the corresponding interval of U (where $U' < U < U^*$) as well as B^* and U^* , is directly related to the experimentally measured magnetic moment M(B). When $B < B^*$, the second Landau subband begins filling up. Its DOS starts with D(U')=0and in a certain interval of B is related to the already determined D(U). The unknown D(U) may again be determined experimentally in the next interval of U. In still weaker B, the third Landau subband switches in, etc. As a result, D(U) may be determined in the whole interval $U' \le U \le U''$. Therefore, M(B) may be calculated (with no adjustable parameters) and compared to the experimental M(B), determining the accuracy of the approach and the region of its validity.

When $B \to \infty$, then $DOS \to \infty$, and all electrons gather in the lowest-energy state: $\epsilon_F(B) \to \frac{1}{2}\hbar \Omega + U'$. In strong enough *B*, only the j=0 Landau subband is occupied. This happens when

$$\epsilon_F(B) = \frac{1}{2}\hbar \,\Omega + U_0 \tag{3b}$$

is less than $\frac{3}{2}\hbar \Omega + U'$, i.e., when

$$\hbar \Omega > U_0(B) - U' \quad . \tag{3c}$$

Then the total number of electrons

$$N = \int_{U'}^{U_0} D(U) \, dU = (2eB/ch) S(U_0) \quad , \tag{4}$$

where $U_0 = \epsilon_F - \frac{1}{2}\hbar \Omega$. The total electron energy

$$E = (2eB/ch) \int_{U'}^{U_0} (\frac{1}{2}\hbar \Omega + U) (\partial S/\partial U) dU .$$

Accounting for Eq. (4),

$$E = N\epsilon_F - (2eB/ch) \int_{U'}^{U_0} S(U) dU \quad . \tag{5}$$

The magnetic moment M = -dE/dB and magnetic susceptibility $\chi = dM/dB$, by Eqs. (3b), (4), and (5), are

$$M = (2e/ch) \int_{U'}^{U_0} SdU - \mu^* N \quad , \tag{6}$$

$$\chi = NU_0'(B)/B \quad , \tag{7}$$

where $\mu^* = e\hbar/2m^*c$. Since $B \to \infty$ yields $U_0 \to U'$, and $M \to -\mu^*N$, so, by Eq. (7),

$$U_{0}(B) - U' = -N^{-1} \int_{B}^{\infty} B' \chi(B') dB'$$

= $-N^{-1} \int B' d(M' + \mu^{*}N)$
= $N^{-1} \int_{B}^{\infty} (M' + \mu^{*}N) dB'$, (8)

while Eq. (3b) provides $\epsilon_F(B)$. By Eq. (1),

$$D(B) = (2eB/ch)S'(U_0) = (2eB/ch)S'(B)/U'_0(B)$$

By Eq. (4), S'(B) = (chN/2eB)', and by Eq. (7), $U'_0(B) = BX/N$. So,

$$D(B) = -N^2 B^2 \chi \quad . \tag{9}$$

Since $D(B) \ge 0$, Eq. (9) may be valid only when $\chi < 0$. Equations (8) and (9) determine (in a parametric form) D(U) directly from experimental data. Equations (4) and (8) determine S(U). By Eqs. (3c) and (8), they are valid when B > B', where B^* is determined by

$$\phi(B^*) \equiv \left| N^{-1} \int_{B^*}^{\infty} B' dM' \right| = \hbar \,\Omega^* \quad . \tag{10}$$

If $\hbar \Omega^* > U'' - U'$, then D(U), S(U) are completely determined. Otherwise, when $B < B^*$, the next j = 1 Landau subband is populated. Consider

$$U_0 - U' < 2\hbar \Omega \quad . \tag{10a}$$

Then, $\epsilon_F = \frac{1}{2}\hbar \Omega + U_0 < (\frac{5}{2}\hbar \Omega + U')$, and other $(j \ge 2)$ Landau subbands are empty. A simple calculation (see also later) replaces Eqs. (4) and (6) by

$$N = (2eB/ch)(S_0 + S_1) , \qquad (11)$$

$$M = (2e/ch) \left(\int_{U'}^{U_0} SdU + \int_{U'}^{U_1} SdU - 2\mu^* BS_1 \right) - \mu^* N, \quad (12)$$

where $S_0 = S(U_0)$, $S_1 = S(U_1)$, and by Eq. (3), $U_1 = U_0 - \hbar \Omega$. As long as $U_1 - U' < \hbar \Omega^*$ the function $S(U_1)$ is known from Eqs. (4) and (8). So Eqs. (11) and (12) are similar to Eqs. (4) and (6):

$$N_1 = N - 2eBS_1 / ch = (2eB/ch)S(U_0) , \qquad (12a)$$

$$M_{1} = M - (2e/ch) \left(\int_{U'}^{U_{1}} SdU - 2\mu^{*}BS_{1} \right)$$

= (2e/ch) $\int_{U'}^{U_{0}} SdU - \mu^{*}N$, (12b)

where N_1 and M_1 are now known. Accounting for Eq. (11), one obtains, similar to Eq. (7),

$$\chi_1(B) \equiv dM_1/dB = U_0'(B)N_1/B \quad , \tag{13}$$

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where $N_1 = N_1(B)$. So, similar to Eq. (8),

$$U_0(B) - U' \equiv \phi_1(B) = -\int_B^\infty B' dM_1' / N_1(B') \quad . \tag{14}$$

Now, by Eq. (11), $D(B) = (2eB/ch)S'(B)/U'_0(B)$. So, accounting for Eq. (12a) [with nonconserved $N_1(B)$] and Eq. (13), one obtains

$$D(B) = (N_1/\chi_1)(N_1/B)'; S(B) = chN_1/2eB$$
. (15)

Equations (14) and (15) determine D(U) in the new interval of U, where $U_1 - U' < \hbar \Omega^*$ (thus, $U_0 - U' < \hbar \Omega^* + \hbar \Omega$), and, by Eq. (10a), $U_0 - U' < 2\hbar \Omega$. By Eq. (14), corresponding magnetic fields $B > B_1^*, B_1$ are determined by

$$\phi_1(B_1^*) = \hbar (\Omega^* + \Omega_1^*); \ \phi_1(B_1) = 2\hbar \Omega_1 \ . \tag{15a}$$

If $B_1^* > B_1$, then for $B > B_1^*$ one proceeds with Eqs. (14) and (15), where S_1 is now determined in a broader interval, and repeats this procedure until one reaches B_1 . If $B_1 > B_1^*$, then one accounts for N, M, χ for the (j = 2) Landau sub-band. General formulas which follow from Eqs. (2) and (3) read

$$N = \sum_{j=0}^{J_1-1} \int_{U'}^{U''} D(U) dU + \sum_{j=J_1}^{J_2} \int_{U'}^{U_j} D(U) dU ;$$

$$E = \sum_{j=1}^{J_1-1} \int_{U'}^{U''} [(j+\frac{1}{2})\hbar \Omega + U] D(U) dU + \sum_{j=J_1}^{J_2} \int_{U'}^{U_j} [(j+\frac{1}{2})\hbar \Omega + U] D(U) dU .$$

So,

$$N = (2eB/ch) \left(j_1 S + \sum_{j_1}^{j_2} S_j \right) , \qquad (16)$$

$$(ch/2e)M = -\mu^* B[2j_1^2 S + \sum_{j=j_1}^{J_2} (2j+1)S_j] + \sum_{j=j_1}^{J_2} \int_{U'}^{U_j} SdU + j_1 \left(\int_{U'}^{U''} SdU + \epsilon_F S - U''S \right) ,$$
(17)

where $S_j \equiv S(U_j) = S[\epsilon_F - (j + \frac{1}{2})\hbar \Omega]$. The subbands with $j = 0, 1, \ldots, j_1 - 1$ are completely filled, while those with $j > j_2$ are completely empty; $j_1 \leq j \leq j_2$ corresponds to partially occupied subbands.⁷

By Eqs. (16) and (17), step by step one determines D(U) in the whole interval (U', U''). Then one may calculate M(B) from Eqs. (16) and (17) in weaker fields and compare it to the experimental M, thus verifying the approach.

Clearly, the main point in the approach is the same *B*-independent S(U) in all Landau subbands. Then the population of every $j \ge 1$ subband starts with U = U' and covers the region of U which has already been determined in higher magnetic fields. The approach is valid when

 $l_0 = (ch/eB)^{1/2}$ is small compared to the characteristic potential range l_U . If this region covers the whole interval $U'' - U' \equiv \Delta U$, i.e., if $\Delta U > \pi^2 \hbar^2 / m^* l_U^2$, then *M* calculated from Eqs. (16) and (17) and experimental *M* agree until $B \sim B_U$, where $l_U \sim l_0(B_U)$.

The best magnetic fields to start the determination of D(U) are those when $U_0 \approx U'$. Then, by Eqs. (3a), (4), and (6),

$$M/N = -\mu^* + \frac{1}{6}B^{-3/2}(chN/2eaS)^{1/2} .$$
 (18)

Above I consider only zero temperature. To account for a finite but low temperature is little problem.

Similar calculations may be performed for heat capacity, or when the total number of electrons N is not exactly conserved (e.g., as suggested by Barraff and Tsui⁸). Suppose, for instance, that the reservoir of electrons preserves ϵ_F . If, e.g., only the j=0 Landau subband is occupied, then B determines $U_0 = \epsilon_F - \frac{1}{2}\hbar \Omega$ and $E(U_0)$. Since

$$E(U_0) = \int_{U'}^{U_0} \left(\frac{1}{2}\hbar \Omega + U\right) D(U) dU$$
$$= \int (\epsilon_F - U_0 + U') D(U) dU ,$$

so

$$E^{\prime\prime}(U_0) = \epsilon_F D^{\prime}(U_0) - D(U_0)$$

This equation determines D(U).

The suggested determination of the DOS is related to two main assumptions. First, that a one-particle DOS is appropriate, i.e., that the electron-electron interaction is small, i.e., $e^2 n^{1/3}/\epsilon_d << \hbar \Omega$, where ϵ_d is the dielectric constant and *n* is the electron density.⁹ The second assumption is $l_0 << a_i$, where a_i is the impurity Bohr radius. When $l_0 << a_i$, the center of cyclotron orbit moves along an equipotential line U = const, and Eq. (1) for DOS is valid. Then, whatever U is,¹⁰ the presented calculation is valid.

All approximations may make the apparent DOS more uniform than it really is.

To summarize: (i) Suppose magnetic moment per electron saturates in experiment to $(M/N) + (e\hbar/m^*c) \propto B^{-3/2}$. Then determine B^* from Eq. (10) and consider $B > B^*$. There simple Eqs. (8) and (9) determine DOS D(U), while Eqs. (4) and (8) yield S(U). (ii) Determine N_1, M_1 by Eqs. (12a) and (12b). Find D(U), S(U) from Eqs. (14) and (15), and (12a) and (12b) in the region of (U-U') from Eq. (15a). If $B_1^* > B_1$, proceed further by Eqs. (14) and (15). If $B_1 > B_1^*$, proceed according to Eqs. (16) and (17). (iii) When D(U) and S(U) are determined in the whole interval (U', U''), compare theoretical M(B) from Eq. (17) with the experimental one. If they deviate at $B \sim B_u$, then the characteristic potential range is $l_u \sim (ch/eB_u)^{1/2}$.

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- ⁷Equation (17), similar to Eqs. (7) and (13), yields kinks in χ , and correspondingly $\chi = 0$, $\chi_1 = 0, \ldots$, when $U'_0 = 0$, i.e., when $U_0 = U', U'', \ldots$ (*B* position is temperature independent), and the subband starts or ends. At sufficiently low temperatures, when these kinks are seen experimentally, one may directly determine the beginning (where $d\chi/dB > 0$) and the end ($d\chi/dB < 0$) of a subband.
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- ⁹Magnetic field, by Eq. (1), increases the density of states. Thus, it decreases the screening length and the relative role of electronelectron interaction.
- ¹⁰To be accurate, it should be determined from the Poisson equation for a given situation of impurities.