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# **Research Article**

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# Temperature and magnetic field effect on the thermodynamic properties of 2DEG

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# Abstract:

A numerical calculation of the temperature and magnetic field dependence of the specific heat capacity, the magnetization, and the chemical potential is carried out. Of particular interest are the properties of the energy of a magnetic field in a two-dimensional electron gas exposed to a magnetic field. Thus, in this paper, we illustrate the effect of temperature on the oscillation dHvA of specific heat capacity and magnetization. As well a mathematical model has been developed for calculating the temperature dependence of the oscillations of the chemical potential and the density of states under the influence of a magnetic field. Using the proposed model, the results were explained at different broadening factors  $\Gamma$ . The calculated results show that specific heat capacity and magnetization increase as the magnetic field increases. Additionally, these increases carry out that the magnetic field is large enough to neglect the mixing of Landau levels caused by the sharp peak of Landeau levels. Moreover, the 2D dHvA effect is characterized by a sawtooth strap at a very low temperature.

**Keywords:** Two-dimensional electron gas, Density of state, Chemical potential, Specific heat capacity, Magnetization, De Haas-van Alphen effect.

#### 1. Introduction:

A thermodynamic property's oscillatory change as a function of magnetic field effect (B) intensity is known as the de Haas-van Alphen (dHvA). The quantization of electron orbits in a constant B intensity is the primary contributor to the dHvA effect. Generally, the electrons have a cyclotron frequency as they circle the magnetic field  $\omega_c = \frac{qB}{m}$ . L. D. Landau first proposed this effect in 1930 [1]. Haas and van Alphen measured it for the first time in the same year [2]. The original theory of the dHvA oscillations of Lifshitz-Kosevich in 1955 was initially demonstrated by 3D metals with magnetization with respect to the magnetic field (B) and temperature for an arbitrary electronic spectrum [3]. The delta-shaped density of states (DOS) of an ideal 2DEG, under a perpendicular B, maybe the cause of the magnetization oscillation [4].

On the side of theoretic examinations, previous reports have demonstrated the Landau levels (LLs) broadening, in the extreme quantum limits and are calculated by self-consistently taking into consideration of scattering of electrons on an impurity potential [5, 6]. Moreover, another work, involving perturbative action of the disorder and interaction of Columb, acquired a DOS with sharp edges in the limit wherever LLs mixing is not considered [7]. Reports on the DOS derived from tests, however, reveal broadened LLs. This is true whether the DOS is obtained from measurements of magnetization [8-10], heat capacity [5, 11], and or capacitance [12-13]. Furthermore, depending on the strength of the applied magnetic field, LLs overlaps may appear, indicating the presence of electronic states among the ideal DOS peaks. This derivation has no localization effects and includes characteristics relating to the impurity design, specifically, its density and distance from the two-dimensional electron systems (2DES) plane. These overlaps have been analytically proven with the existence of a weak disorder [14].

In a two-dimensional electron gas, it is essential to investigate the effect of the magnetic field and temperature on the thermodynamic properties. Information about the electron density can be obtained from 2D thermodynamic properties. In addition, chemical potential, specific heat capacity, and magnetization may be acquired by focusing the electron density as a constant.

Herein, we investigate the magnetic field and temperature effect on the thermodynamic features of LLs in GaAs 2D electron gas. The effect of oscillation dHvA in 2D electron gas is studied in this work. This effect is supported by numerical simulations of chemical potential and magnetization. The 2D dHvA effect is characterized. A numerical evaluation and discussion of the influence of temperature and a magnetic field are discussed.

#### 2. Theoretical Model and formulation:

The impurity Hamiltonian under the influence of an applied magnetic field at room temperature, the computing process, and the magnetic characteristics are all shown in this section.

#### 2.1 The Energy:

The energy without a magnetic field,  $E = \frac{\hbar^2 k^2}{2m^*}$ , is specified by solving the timedependent Schrödinger equation in one dimension for the free particle:

$$-\frac{\hbar^2}{2m^*}\frac{\partial^2\Psi(x,t)}{\partial x^2} = i\hbar\frac{\partial\Psi(x,t)}{\partial t}$$
(1)

where,  $m^*$  is the electron's effective mass.

Then, we are interested in the calculation of the energy of a charged particle in a magnetic field. This can be achieved by solving the Schrodinger wave equation [15, 16]. The Hamiltonian of the Landau system is given by:

$$\widehat{H} = \frac{1}{2m} \left( \,\widehat{p} - q\,\overrightarrow{A} \right)^2 \tag{2}$$

where,  $\hat{p}$  is the momentum operator and  $\vec{A}$  is the vector potential related to the B introduced in the z-direction. By choosing a gauge such as,  $\vec{A} = B_z x \hat{y}$ , the wave function takes the following form [15, 17]:

$$\psi(x) = e^{ik_y y + ik_z z} \phi(x) \tag{3}$$

Where,  $\phi(x)$  is a solution to the harmonic oscillator equation. Taking a count for, the time-Independent Schrödinger equation [18]:

$$\left[\frac{1}{2m}\left(\hat{P}_x^2 + \left(\hbar k_y - qB_z x\right)^2\right) + \frac{\hbar^2 k_z^2}{2m}\right]\phi(x) = E\phi(x) \tag{4}$$

where the term  $\frac{\hbar^2 k_Z^2}{2m}$  is the kinetic energy in the Z-direction. The total energy is defined as the sum of particle energy in the x-y plane and the kinetic energy in the Z-direction:

$$E = E_n + \frac{\hbar^2 k^2}{2m} \tag{5}$$

where the Hamiltonian for the harmonic oscillator takes this form [15]:

$$H = \frac{\hat{P}_x^2}{2m} + \frac{m}{2}\omega_c^2 (x - k_y l_c^2)^2$$
(6)

where  $l_c$  is the magnetic length, and  $\omega_c = \frac{q_B}{m}$  is the electron cyclotron frequency.

And the n<sup>th</sup> LLs is obtained as [19]:

$$E_n = \hbar\omega_C \left( n + \frac{1}{2} \right) \tag{7}$$

Thereafter, it is straightforward to calculate the thermodynamic features of LLs in GaAs, a 2D electron gas, and study the effects of a magnetic field and temperature on these properties.

#### 2.2 The density of state:

The DOS of the two-dimensional electron gas (2DEG) is given as a sequence of delta functions [20]:  $D(E) = D_0 \sum_n \delta(E - E_n)$ . Herein, we take the case when the broadening factor is kept at a constant value, and we introduce the Gaussian form [21]:

$$D(B,E) = \frac{eB}{\pi\hbar} \sum_{n} \frac{1}{\sqrt{2\pi}\Gamma} exp\left(-\frac{(E-E_n)^2}{2\Gamma^2}\right)$$
(8)

Where e is the electron charge,  $\hbar$  is Planck's constant/ $2\pi$ ,  $\Gamma$  is the broadening parameter, and  $E_n$  is the energy of the LLs, which was shown in Eq. (7) [20].

#### 2.3 Chemical potential:

Chemical potential is the change in energy of a thermodynamic system when a new particle is added while the entropy and volume remain constant [22]. To determine the chemical potential, we employ the electron concentration (N), which is given by:

$$N = \int_{0}^{+\infty} f(E, \mu, T) D(B, E) \, dE$$
(9)

Where  $\mu = \mu$  (*B*, *T*) is the chemical potential, D(B, E) is the Gaussian DOS for two-dimensional electron systems, which is given in equation (12), and  $f(E, \mu, T)$  is the Fermi-Dirac distribution function [23], which is given in this relation:

$$f(E,\mu,T) = \frac{1}{1 + exp\left[\frac{(E-\mu)}{k_B T}\right]}$$
(10)

In addition, chemical potential can be calculated using a root-finding approach by using the electron concentration (N) as a constant. As an experimental result, the electron concentration is set at  $3.6 \times 10^{11} cm^{-2}$  to simulate conditions similar to those in experiments [21, 22]. So, the chemical potential  $\mu$  oscillates with respect to B and is periodic concerning the filling factor. Where the LLs filling factor v is the number of electrons per LLs at a given magnetic field [21, 24] degeneracy, which is mathematically given as:  $v = \frac{hN}{eB}$ 

# 2.4 Magnetization:

The magnetization of the system can be calculated from the free energy F at constant electron concentration N using the following relationship [21]:

$$M(B,T) = -\frac{\partial F}{\partial B}\Big|_{N=constant}$$
(11)

Where:

$$F = \mu N - k_B T \int_{0}^{+\infty} D(B, E) \ln \left( 1 + \exp \left[ \frac{\mu - E}{k_B T} \right] \right) dE$$
(12)

Once the chemical potential and the DOS are known, it is possible to predict how these magneto-thermodynamic properties will behave. Finally, the magnetization becomes:

$$M = -\frac{ekT}{\pi\sqrt{2\pi}\hbar\Gamma} \frac{\int_{0}^{\infty} \frac{\sum_{n} exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)}{1+exp\left(\frac{E-\mu}{kT}\right)} dE \int_{0}^{\infty} \frac{\sum_{n} exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)}{1+exp\left(\frac{E-\mu}{kT}\right)} dE} + \frac{\int_{0}^{\infty} \frac{\sum_{n} exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) exp\left(\frac{E-\mu}{kT}\right)}{\left(1+exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE} + \frac{e^{2}kTB}{\pi\sqrt{2\pi}\hbar\Gamma} \int_{0}^{\infty} \frac{\sum_{n} exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)}{\int_{0}^{\infty} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) exp\left(\frac{E-\mu}{kT}\right)}{\left(1+exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE} + \frac{e^{2}kTB}{\pi\sqrt{2\pi}\hbar\Gamma} \int_{0}^{\infty} \sum_{n} exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) ln\left(1+exp\left(\frac{\mu-E}{kT}\right)\right) dE + \frac{e^{2}kTB}{\pi\sqrt{2\pi}\Gamma^{3}m} \int_{0}^{\infty} \sum_{n} \left(n+\frac{1}{2}\right) (E-E_{n}) exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) ln\left(1+exp\left(\frac{\mu-E}{kT}\right)\right) dE + \frac{e^{2}kTB}{\pi\sqrt{2\pi}\Gamma^{3}m} \int_{0}^{\infty} \left(13\right) \frac{1}{2} \left(E-E_{n}) exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) ln\left(1+exp\left(\frac{\mu-E}{kT}\right)\right) dE - \int_{0}^{\infty} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) ln\left(1+exp\left(\frac{E-E_{n}}{kT}\right)\right) dE - \int_{0}^{\infty} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) ln\left(1+exp\left(\frac{E-E_{n}}{kT}\right)\right) ln\left(1+exp\left(\frac$$

$$\frac{\frac{ekT}{\pi\sqrt{2\pi}\hbar\Gamma} \int_{0}^{\infty} \frac{\sum_{n} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)}{1+exp\left(\frac{E-\mu}{kT}\right)} dE}{\left(1+exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE} \int_{0}^{\infty} \frac{\sum_{n} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)exp\left(\frac{\mu-E}{kT}\right)}{\left(1+exp\left(\frac{\mu-E}{kT}\right)\right)^{2}} dE} - \frac{\frac{e^{2}kTB}{\pi\sqrt{2\pi}\Gamma^{3}m} \int_{0}^{\infty} \frac{\sum_{n} \frac{(n+\frac{1}{2})(E-E_{n})exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)}{1+exp\left(\frac{E-\mu}{kT}\right)} dE}}{\int_{0}^{\infty} \frac{\sum_{n} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)exp\left(\frac{\mu-E}{kT}\right)}{\left(1+exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE}}{\int_{0}^{\infty} \frac{\sum_{n} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)exp\left(\frac{\mu-E}{kT}\right)}{\left(1+exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE}}{\int_{0}^{\infty} \frac{\sum_{n} \frac{exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)exp\left(\frac{E-\mu}{kT}\right)}{\left(1+exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE}$$

# 2.5 Specific Heat capacity:

The specific heat capacity of two-dimensional electron systems is the quantity of heat energy required to increase the temperature of a determined amount of matter [25]. Its expression for the constant volume of an electron gas is provided by:

$$C_{v}(B,T) = \frac{\partial U}{\partial T}$$
(14)

where U is internal energy, which in this situation is given in the form [21, 23]:

$$U = \int_{0}^{\infty} D(B, E) f(E, \mu, T) (E - \mu) dE$$
 (15)

where  $f(E, \mu, T) = \frac{1}{1 + exp\left[\frac{(E-\mu)}{k_B T}\right]}$  is the Fermi-Dirac distribution function,

 $\mu=\mu$  (B, T) is the chemical potential,  $k_B$  is the Boltzmann's constant, and D(B, E) is the DOS. Finally, the specific heat capacity becomes:

$$C_{v}(B,T) = -\frac{eB}{kT^{2}\pi\hbar\Gamma\sqrt{2\pi}} \int_{0}^{\infty} \frac{(E-\mu)\sum_{n} \exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) \exp\left(\frac{E-\mu}{kT}\right)}{\left(1+\exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE \int_{0}^{\infty} \frac{(E-\mu)\sum_{n} \exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) \exp\left(\frac{E-\mu}{kT}\right)}{\left(1+\exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE + \frac{eB}{kT^{2}\pi\hbar\Gamma\sqrt{2\pi}} \int_{0}^{\infty} \frac{\left(E-\mu\right)^{2}\sum_{n} \exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right) \exp\left(\frac{E-\mu}{kT}\right)}{\left(1+\exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE + \frac{eB}{\pi\hbar\Gamma\sqrt{2\pi}} \int_{0}^{\infty} \frac{\sum_{n} \exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)}{\left(1+\exp\left(\frac{E-\mu}{kT}\right)\right)^{2}} dE + \frac{eB}{\pi\hbar\Gamma\sqrt{2\pi}} \int_{0}^{\infty} \frac{\sum_{n} \exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)}{\left(1+\exp\left(\frac{E-\mu}{kT}\right)^{2}\right)} dE + \frac{eB}{\pi\hbar\Gamma\sqrt{2\pi}} \int_{0}^{\infty} \frac{\sum_{n} \exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E-\mu}{kT}\right)}{\left(1+\exp\left(\frac{E-\mu}{kT}\right)^{2}\right)} dE + \frac{eB}{\pi\hbar\Gamma\sqrt{2\pi}} \int_{0}^{\infty} \frac{\exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E-\mu}{kT}\right)}{\left(1+\exp\left(\frac{E-\mu}{kT}\right)^{2}}\right)} dE + \frac{EB}{\pi\hbar\Gamma\sqrt{2\pi}} \int_{0}^{\infty} \frac{\exp\left(-\frac{(E-E_{n})^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E-\mu}{kT}\right)} \frac{EB}{\pi\hbar\Gamma\sqrt{2\pi}} dE + \frac{EB}{\pi} \int_{0}^{\infty} \frac{E^{2}}{2\Gamma^{2}} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \frac{EB}{\pi} \int_{0}^{\infty} \frac{E^{2}}{2\Gamma^{2}}} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \frac{E^{2}}{2\Gamma^{2}} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \frac{E^{2}}{2\Gamma^{2}} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \frac{E^{2}}{2\Gamma^{2}} \exp\left(-\frac{E^{2}}{2\Gamma^{2}}\right)} \exp\left(-\frac{E^{$$

In this study, no spin–splitting is considered. The effective mass employed here corresponds to 0.0667 me, wherever me is the mass of the electron.

#### 3. Results and Discussion:

Here, in this part, we demonstrate the results of a study of the thermodynamic features of LLs in GaAs, a 2D electron gas. Figure 1 shows the variation curves in two graphs for energy E versus wave vector k. In the left graph, the varying k values range from 0 to  $10^{10}$ , while in the right graph, we took k values ranging from  $-2 \times 10^9$  to  $2 \times 10^9$ . We found that, in all cases, the energy of an electron in GaAs increases with wave vector k due to symmetry and has a quadratic relationship with the wave vector [26,27].



Figure1: The energy E versus wave vector k curve for an electron inside.

In Figure 2, the energy E has been plotted against B for different values of n, which vary from 1 to 10. We notice that the spaces between the LLs increase with the magnetic field B. We also noted that for a fixed value of B, the energy levels of the harmonic oscillator increase as n increases [28, 29,30].

Figure 3 displays the DOS as a function of energy for two different values of the broadening parameter:  $\Gamma = 0.2 \text{ meV}$  and  $\Gamma = 0.6 \text{ meV}$ , using equation (8). We notice that the DOS is obviously affected by the imperfection of the samples considered [27. 30].



Figure2: Energy diagram of the Landau levels for a two-dimensional electron gas in the presence of a magnetic field B.

Figure 4 shows a plot of the DOS of 2DEG in GaAs as a function of electron energy E, calculated for a magnetic field B varying between 0.2T and 10T and for three different broadenings. The sharp peaks of the LLs begin to smooth out as the magnetic field increases [27, 31]. We can also assume that the magnetic field is large enough to neglect the mixing of LLs due to disorder.



**Figure3:** Density of state for a broadening  $\Gamma$ =0.2meV (a) and  $\Gamma$ =0.6meV (b).



Figure 4: Density of state calculated for a field B varying between 0.2T and 10T and for broadening  $\Gamma$ =0.2meV,  $\Gamma$ =0.6meV and  $\Gamma$ =0.8meV.

The chemical potential oscillates with respect to B in the absence of LLs broadening, with sharp peaks appearing at even filling factors v. Where, the filling factor v is the number of electrons per LLs degeneracy which is provided by  $v = \frac{hN}{eB}$ . This indicates that to add one more electron, one must move to the level above since the last inhabited LLs are already completely filled for even v. On the other hand, an odd v, refers to a level that was last occupied and filled to half its degeneracy. In figure 5, we present the chemical potential  $\mu$  with respect to B that is periodic concerning the filling factor, at a fixed temperature T = 0.5 K for a broadening factor  $\Gamma$ =0.3meV. We notice that the chemical potential displays sharp peaks for each even filling factor v without LLs broadening, at very low temperatures [21, 24]. However, as the temperature rises and an LLs broadening is introduced, the sharpness of the oscillations softens and decreases [32, 33].



Figure 5: Chemical potential as a function of magnetic field at temperature T= 0.5 K and for a broadening factor  $\Gamma$ =0.3meV.

Now we are interested in the effect of the B on specific heat capacity. We display in Figure 6 the variation of specific heat capacity with a B at two different values of the temperature. The study of DOS exhibits a periodic oscillation credited to the development of the disorder. This behavior of oscillatory is shown also in figure 6 of the heat capacity [25].



Figure 6: Oscillation of heat capacity  $C_v$  as a function of the magnetic field B at constant broadening factor  $\Gamma$  for different temperature

Figure 7 displays the relationship between the heat capacity and temperature for three dissimilar values of the B. We evidence that whatever the B, there is a critical temperature that is at T = 3.5 K, and at this critical temperature, the heat capacity achieves its maximum, and we can say at this point that the system has stored the most energy. Outside of that critical temperature, the heat capacity decreases with the B because, as the temperature increases, the heat capacity becomes less sensitive to field changes and the particles are more stable.



Figure 7: Heat capacity as a function of temperature for a GaAs two-dimensional electron gas.

After studying, the chemical potential, we determine the exact expression for the thermodynamical potential to investigate the magnetization of the system. Then we demonstrate the results of Eq. (13) in Figure 8. We display the magnetization versus B for two different values of the temperature: T = 0.3 k and T = 5 k, at a fixed broadening factor  $\Gamma = 1 \text{ meV}$ . It is clear that magnetization oscillates with respect to B strength and inclines to be zero at low field strengths, closely following the oscillation of the chemical potential. At low temperatures, the magnetization shows a dHvA oscillation that resembles a sawtooth [27, 28, 29]. Our results supported the numerical finding in Reference [25, 33].



Figure 8: Magnetization as a function of magnetic field at broadening factor  $\Gamma = 1 \text{ meV}$ for temperature T=0.3K and T=5K.

#### 4. Conclusions:

In conclusion, we have solved the Hamiltonian of an electron in a two-dimensional electron's gas, under the effect of an external magnetic field and temperature. In 2D electron systems, the effect of temperature and LLs broadening is taken into account involving a Gaussian-shaped DOS. The broadening values that were taken into consideration took on a variety of shapes, including various constant factors, a square-root dependence on the B, and an oscillating function about the filling factor v. Whatever the form, the acquired B performance of the chemical potential, specific heat capacity, and magnetization reveal the same tendency. The broadening only affects the oscillations width of the B for individual interlevel and internal-level contribution. It is found that the 2D electron systems obtain their ideal electron gas features at a specified temperature. Under this defining temperature, the LLs broadening has no further effect on how the thermodynamic properties behave.

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