Temperature Dependence of the Occupancy of Landau Subbands in a Two-Dimensional Electron Gas

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Numerical modeling has been used to study the temperature dependence of the chemical potential and the occupation of the Landau subbands in a two-dimensional electron gas. Calculations were performed for various values of the filling factor ν, taking into account the level broadening due to scattering events. Graphs depicting the temperature dependence of the electron concentration within the Landau subbands were constructed. These dependencies enable the analysis of the thermal excitations of electrons between subbands. Additionally, a simple model was used to identify the thermal excitations of electrons within a single subband.

topics: heterostructure, quantum well, two-dimensional electron gas, Landau levels

1. Introduction

When the magnitude of the magnetic field applied perpendicular to the plane of the quantum well changes, several thermodynamic properties of the two-dimensional (2D) electron gas undergo abrupt changes. These changes manifest themselves as oscillations in various thermodynamic quantities of the 2D electron gas, such as magnetoresistance, susceptibility, chemical potential, magnetization, heat capacity, and others [1–11]. From these observed oscillations, critical information about the band parameters of the structure can be derived, including effective mass, carrier concentration, spin splitting and etc.

To date, a substantial number of theoretical calculations have been performed to study the thermodynamic properties of a two-dimensional (2D) electron gas. These studies focus on how these properties vary with the magnitude of the magnetic field B, the temperature T, the electron concent ration in the quantum well n_S, and the level broadening Γ, as detailed in references [12–21]. Generally, such calculations necessitate the use of numerical methods.

Of particular interest are the changes in thermodynamic quantities with temperature at a fixed value of the magnetic field. In this case, the conduction band consists of several Landau subbands (Fig. 1). The width of these subbands is approximately of the order of 2Γ, and the distances between the centers of the subbands are equal to $\hbar\omega$ ($\hbar\omega \sim B$). Typically, in strong fields, where $\hbar\omega > 2\Gamma$, the subbands do not overlap. Depending on the values of the concentration n_S (as well as the temperature and magnetic field), the subbands can be partially or fully occupied.

Theoretical studies [13–15, 17, 18] suggest that at sufficiently low temperatures, where $k_{\mathrm{B}}T \ll 2\Gamma$ and if the Landau subband is only half-filled, the chemical potential of the 2D electron gas remains independent of temperature. In this regime, the heat capacity $C_S(T)$ of the gas behaves similarly to that of a "metallic" system, increasing linearly with temperature. As the temperature increases and approaches $k_{\mathrm{B}}T \sim 2\Gamma$, the heat capacity reaches a saturation point and exhibits a maximum (peak). With further increases in temperature, the heat capacity decreases. These peaks are attributed to intralevel thermal excitations (thermal excitations within the same subband). In the case of weaker magnetic

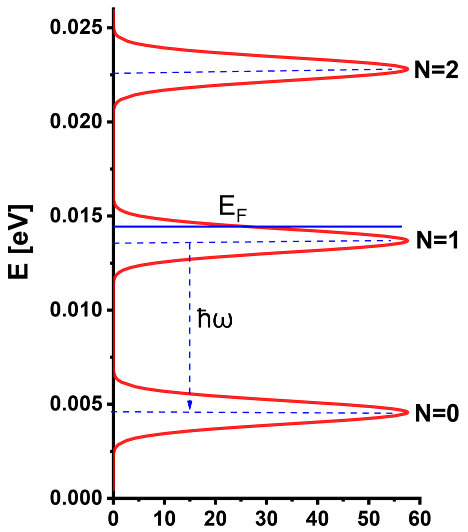

Fig. 1. Energy diagram of the Landau subbands. The density of states $D(E)$ is described by a Gaussian distribution with half-width $\Gamma = 0.6$ meV, effective mass $m^* = 0.023\,m_0$ (for InAs) and total 2D electron concentration $n_S = 0.156 \times 10^{12}$ cm^{-2}; filling factor $\nu = 1.8$ corresponds to a magnetic field $B = 1.81$ T. The first three Landau levels E_N ($N = 0, 1, 2$) are represented by horizontal dashed lines at 0.00456, 0.0137, and 0.0228 eV, respectively. Given these parameters, the Fermi energy (solid horizontal line) is 0.0142 eV.

fields, where $k_\mathrm{B}T \sim \hbar\omega$, interlevel thermal excitations (between different subbands) of electrons are also possible. These interlevel excitations manifest themselves as relatively narrow peaks in the temperature dependence of $C_S(T)$. Such characteristics of heat capacity are corroborated by theoretical calculations and are consistent with experimental observations [4, 13].

In metals, the width of the conduction band is large, typically on the order of several eV. In contrast, the Landau subbands have a much smaller width of $\approx 2\Gamma$ (~ 1 meV), which limits the ability of the electron gas to absorb thermal energy. This characteristic of the electron gas in partially filled Landau subbands should also be reflected in the temperature dependence of other thermodynamic quantities, such as entropy $S(T)$, total energy $U_S(T)$, magnetization $M_S(T)$, and others.

This work investigates a straightforward problem — the temperature dependence of electron concentration in Landau subbands $n_L(N,T)$. This problem has been studied previously in [21]. However, the observed dependence $n_L(N,T)$ is exclusively due to inter-subband thermal excitations of electrons. To identify intralevel thermal excitations within a single Landau subband, we divide the partially filled subband into several sections. Calculation of the temperature dependence of the occupancy of these sections reveals the intralevel thermal excitations. Here, a simpler problem is considered — the partially filled subband is divided into two parts. The first part extends from the bottom of the subband to the Fermi energy, $-\infty, \ldots, E_\mathrm{F}$, and the upper part covers the region $E_\mathrm{F}, \ldots, \infty$. In addition to the occupancy of the subband, the temperature dependence of the gas chemical potential $\mu(T)$ for various values of the filling factor ν is also studied. The correlations between these dependencies are discussed.

2. Model of the Landau level population as a function of temperature

Only the first subband of the spatial quantization of the electron in the quantum well is considered. When a magnetic field is applied perpendicular to the plane of the quantum well, the two-dimensional electron spectrum transforms into Landau levels. For a given total concentration n_S, the chemical potential $\mu(T,B,\Gamma)$ of the 2D electron gas can be determined from the equations

$$n_S = \sum_{N=0}^{\infty} n_L(N,T),$$

$$n_L(N,T) = D\hbar\omega \int_{-\infty}^{\infty} \frac{\mathrm{d}E}{\sqrt{2\pi}\Gamma} \frac{\exp\left(-\frac{(E-E_N)^2}{2\Gamma^2}\right)}{\exp\left(\frac{E-\mu}{k_\mathrm{B}T}\right)+1}. \tag{1}$$

Here, $n_L(N,T)$ represents the concentration of electrons belonging to the N-th Landau level, and E_N denotes the Landau energy levels (spin splitting of the level is not considered)

$$E_N = \left(N + \frac{1}{2}\right)\hbar\omega,$$

$$\hbar\omega = \hbar\frac{eB}{m^*} = \frac{1.16 \times 10^{-4}}{m^*/m_0} B \left[\frac{\mathrm{eV}}{\mathrm{T}}\right], \tag{2}$$

where m^* denotes the effective mass of the electron and m_0 — the rest mass of the electron. In (1), D is the two-dimensional density of states of the subband in the absence of a magnetic field, which is related to $\hbar\omega$ as

$$D\hbar\omega = \frac{eB}{\pi\hbar}, \quad D = \frac{m^*}{\pi\hbar^2} = \frac{m^*}{m_0}\frac{413 \times 10^{12}}{[\mathrm{eV\ cm}^2]}. \tag{3}$$

The filling factor is defined as

$$\nu = \frac{n_S}{D\hbar\omega}. \tag{4}$$

If the temperature is held constant ($T = $ const), the oscillation of the chemical potential $\mu(B)$ can be determined from (1). Conversely, if the magnetic field is held constant ($B = $ const), the dependencies of the chemical potential $\mu(T)$ on temperature can be found.

When inter-subband thermal transitions occur, the electrons concentration of within the Landau subband $n_L(N,T)$ changes with temperature. The

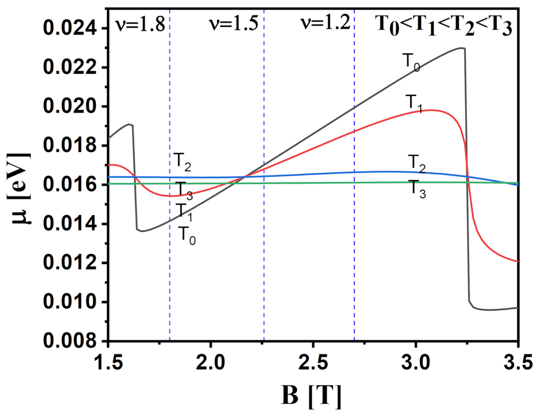

Fig. 2. Magnetic oscillation of chemical potential for various temperatures $k_{\mathrm{B}}T/(2\Gamma) \approx 0, 1, 3, 5$ and $n_S = 0.156 \times 10^{12}$ cm^{-2}, $\Gamma = 0.6$ meV.

most significant thermal transitions (both within and between subbands) occur near the Fermi level. It is evident that at sufficiently low temperatures $k_{\mathrm{B}}T \ll 2\Gamma$, the intra-subband concentration $n_L(N,T)$ remains unchanged with temperature. To investigate the intra-subband thermal excitations of electrons, we divide the concentration of the unoccupied subband (assume this to be the second subband $N = 1$) into two parts

$$n_L(1,T) = n_{LUp}(1,T) + n_{LDn}(1,T), \tag{5}$$

where

$$n_{LUp}(1,T) = D\,\hbar\omega \int\limits_{E_{\mathrm{F}}}^{\infty} \frac{\mathrm{d}E}{\sqrt{2\pi}\Gamma} \frac{\exp\left(-\frac{(E-E_N)^2}{2\Gamma^2}\right)}{\exp\left(\frac{E-\mu}{k_{\mathrm{B}}T}\right)+1},$$

$$n_{LDn}(1,T) = D\,\hbar\omega \int\limits_{-\infty}^{E_{\mathrm{F}}} \frac{\mathrm{d}E}{\sqrt{2\pi}\Gamma} \frac{\exp\left(-\frac{(E-E_N)^2}{2\Gamma^2}\right)}{\exp\left(\frac{E-\mu}{k_{\mathrm{B}}T}\right)+1}. \tag{6}$$

Now, at low temperatures $k_{\mathrm{B}}T \ll 2\Gamma$ even when $n_L(1,T) = \text{const}$, the quantities $n_{LUp}(1,T)$ and $n_{LDn}(1,T)$ vary with temperature. These dependencies characterize the intra-subband thermal excitations.

3. Numerical results and discussion

For numerical modeling, we assume that the partially filled subband will be designated as the $N = 1$ level. The material parameters used for numerical calculations are provided in Fig. 1. The oscillation of the chemical potential corresponding to the interval $1 < \nu < 2$ is depicted in Fig. 2. The filling factor of the underfilled subband $\nu = 1.8$ corresponds to the magnetic field $B = 1.81$ T, while the weakly filled subband $\nu = 1.2$ corresponds to $B = 2.71$ T. The subband is exactly half-filled at $\nu = 1.5$ ($B = 2.17$ T). Calculations were performed for four fixed temperature values: $k_{\mathrm{B}}T_0/(2\Gamma) \approx 0$, $k_{\mathrm{B}}T_1/(2\Gamma) \approx 1$, $k_{\mathrm{B}}T_2/(2\Gamma) \approx 3$, $k_{\mathrm{B}}T_3/(2\Gamma) \approx 5$. The latter two temperature values lead to a complete smearing of the oscillations.

In the case of a weakly filled subband ($\nu = 1.2$), the chemical potential μ decreases monotonically with increasing temperature. For a half-filled subband ($\nu = 1.5$), there is a fixed point where the chemical potential remains independent of temperature as long as $T \ll T_3$. However, with further increase in temperature, the chemical potential μ shifts downward. In contrast, for the underfilled subband ($\nu = 1.8$), the shift in the chemical potential is non-monotonic, unlike the case of $\nu = 1.2$.

To uncover the reasons behind these patterns, we constructed graphs showing the dependence of the chemical potential on temperature for a partially filled subband with $N = 1$ for different values of the filling factor $\nu = 1.8, 1.5, 1.2$. The obtained plots are presented in Fig. 3, where the Fermi energy is located near the first Landau level.

Let us first discuss the case of a partially filled subband (Fig. 3a with $\nu = 1.8$). At low temperatures $k_{\mathrm{B}}T < 2\Gamma$, the chemical potential of the gas increases with temperature. This behavior is also characteristic of one-dimensional systems, where the density of states $D(E)$ decreases with increasing energy. As the temperature continues to increase and $k_{\mathrm{B}}T > 2\Gamma$, the dependence $\mu(T)$ saturates. We propose that this saturation is likely related to the limitation of intra-level thermal transitions due to the finite width of the subband. In this context, inter-level thermal transitions are still exponentially suppressed [21] since $k_{\mathrm{B}}T < \hbar\omega$. It is only in the temperature range where $k_{\mathrm{B}}T \geq \hbar\omega$, i.e., when active interlevel thermal transitions begin, that the chemical potential decreases significantly. The red circular points on the $\mu(T)$ curve correspond to the temperatures $T_0 < T_1 < T_2 < T_3$, which are also indicated in Fig. 2.

In the case of a half-filled subband (Fig. 3b with $\nu = 1.5$), the chemical potential remains temperature-independent until the inter-subband thermal transitions become dominant. As a result, there is a redistribution of electrons, causing the chemical potential to shift downward. This shift is also evident in Fig. 2 at temperature T_3.

For the weakly filled subband ($\nu = 1.2$), the density of states $D(E)$ increases with energy. Similar to the three-dimensional Fermi gas (where $D(E) \sim \sqrt{\varepsilon}$), the chemical potential decreases as the temperature increases.

Thus, the anomalies in the temperature dependence of the chemical potential, as shown in Figs. 2 and 3, are related to the energy dependencies of the density of states (causing the shift in $\mu(T)$) and the finite width of the subband (leading to saturation of $\mu(T)$).

As the temperature changes, the relative occupancy of the Landau subband changes.

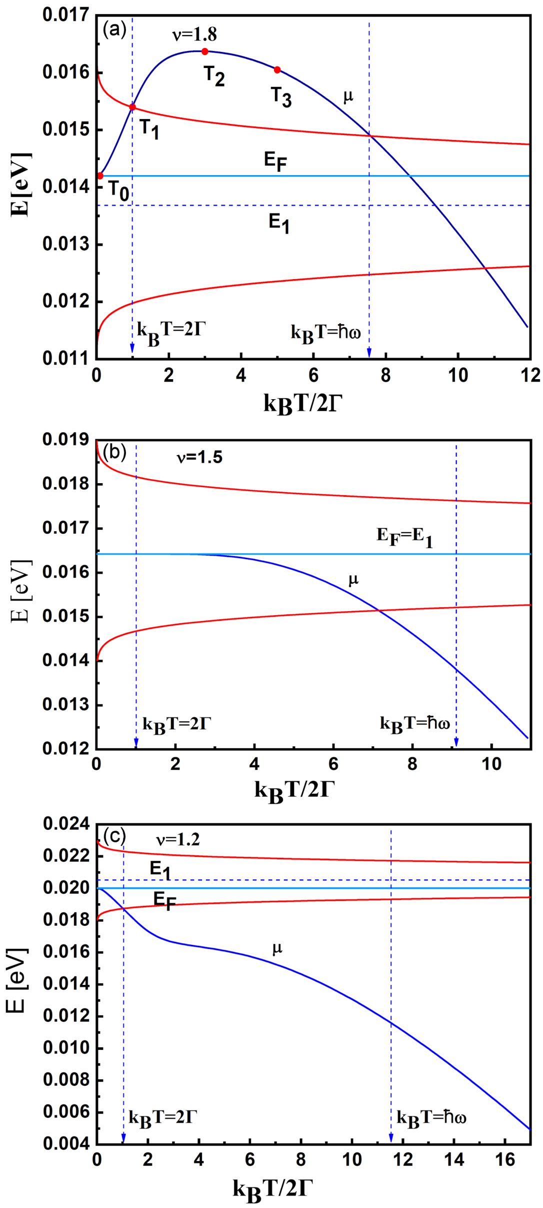

Fig. 3. Variation of chemical potential with temperature for a partially filled subband with $N = 1$: (a) $\nu = 1.8$, (b) $\nu = 1.5$, (c) $\nu = 1.2$ and $n_S = 0.156 \times 10^{12}$ cm^{-2}, $\Gamma = 0.6$ meV.

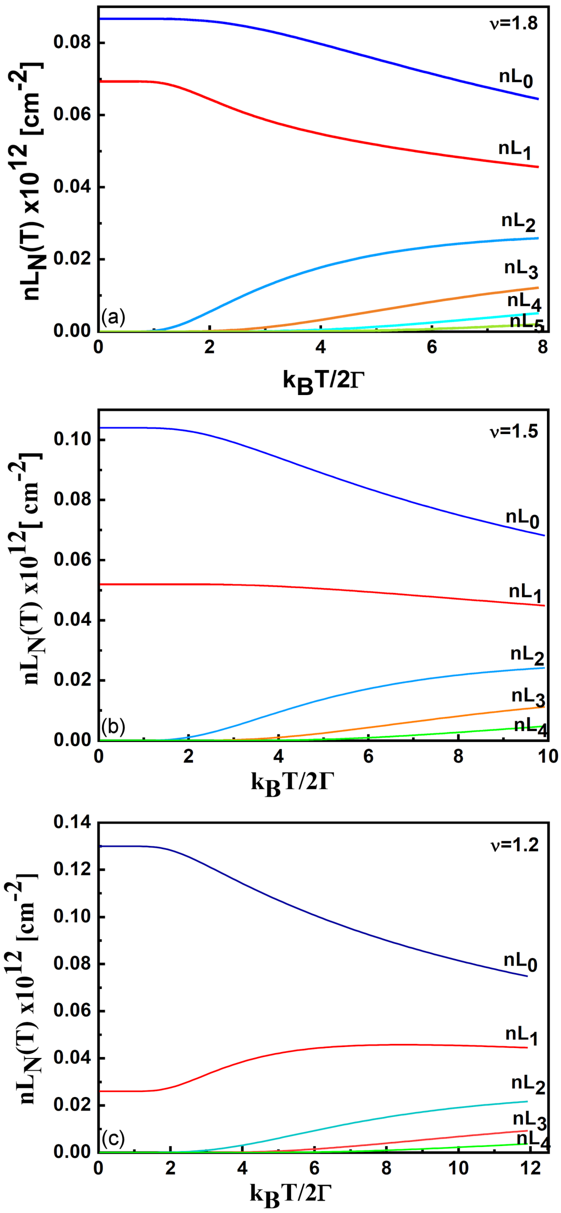

Fig. 4. Temperature dependence of the occupancy of the Landau subbands $N = 0, 1, 2, 3, \ldots$: (a)$\nu = 1.8$, (b) $\nu = 1.5$, (c) $\nu = 1.2$, $n_S = 0.156 \times 10^{12}$ cm^{-2} and $\Gamma = 0.6$ meV.

Using (1), we can determine the occupancy of each level as a function of T and ν. The graphs of these dependencies are presented in Fig. 4, where the Fermi energy is close to the first Landau level. At low temperatures $k_{\mathrm{B}}T < 2\Gamma$, the concentration of electrons in any individual Landau subband remains unchanged, regardless of the filling factor value: (a) $\nu = 1.8$, (b) $\nu = 1.5$ and (c) $\nu = 1.2$. This indicates the absence of inter-subband thermal redistribution of electrons, and although intra-subband transitions exist, they are not discernible in these graphs. A clear inter-subband redistribution occurs at higher temperatures, $k_{\mathrm{B}}T \gg 2\Gamma$. Transitions are observed from the ground subband ($N = 0$) to higher subbands, i.e., nL_0 decreases, while $nL_2, nL_3, nL_4, nL_5, \ldots$ increase. However, the dependencies $nL_1(T)$ for cases: (a) $\nu = 1.8$, (b) $\nu = 1.5$ and (c) $\nu = 1.2$ are different. In the case of a partially filled subband (Fig. 4a with $\nu = 1.8$) for $k_{\mathrm{B}}T > 2\Gamma$, the concentration $nL_1(T)$ decreases, while nL_2 increases with temperature. The increase in nL_2 compensates the decrease in $nL_1(T)$ and $nL_0(T)$. This may be related to the energy differences $(E_2 - \Gamma) - E_{\mathrm{F}} < E_{\mathrm{F}} - (E_0 + \Gamma)$, as well as to the behavior of the chemical potential (see Fig. 3a). A similar interpretation applies to the case of the partially filled subband in Fig. 4c, where $(E_2 - \Gamma) - E_F > E_F - (E_0 + \Gamma)$.

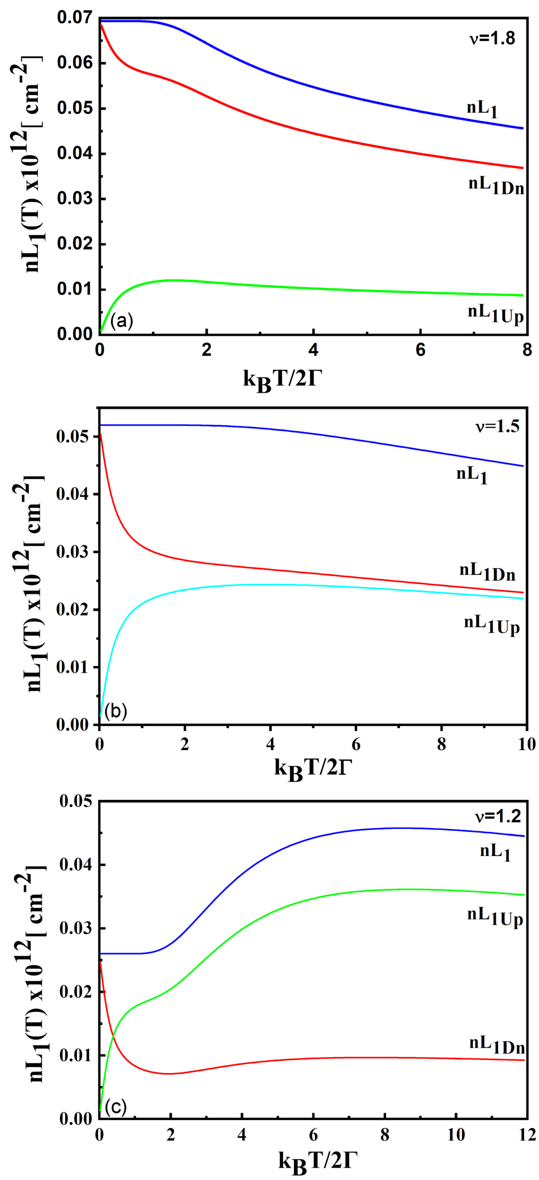

Fig. 5. Temperature dependence of the occupancy for the upper and lower parts of the Landau subband with $N = 1$ at different filling factors: (a) $\nu = 1.8$, (b) $\nu = 1.5$, (c) $\nu = 1.2$ and $n_S = 0.156 \times 10^{12}$ cm^{-2}, $\Gamma = 0.6$ meV.

Figure 5 shows the temperature dependence of the occupancy of the upper and lower parts of the Landau subband with the index $N = 1$. From these dependencies, it is observed that at low temperatures $k_{\mathrm{B}}T < 2\Gamma$ the overall electron concentration within the Landau subband $nL_1(T)$ does not change. However, the concentrations of its upper $nL_{1Up}(T)$ and lower $nL_{1Dn}(T)$ parts do change. This relationship can be expressed as $nL_1(T) = nL_{1Up}(T) + nL_{1Dn}(T)$. This phenomenon is indicative of intra-level thermal transitions within the subband. At higher temperatures $k_{\mathrm{B}}T > 2\Gamma$, the contributions from inter-level thermal transitions between subbands also become significant.

4. Conclusions

When the Landau subbands in a two-dimensional electron gas are sufficiently separated from each other, i.e., $\hbar\omega > 2\Gamma$, the absorption of thermal energy by the system follows different scenarios depending on the relationship between the three parameters $k_{\mathrm{B}}T$, $\hbar\omega$ and 2Γ. These patterns have been directly observed in experimental and theoretical studies of heat capacity [11, 13]. The mechanisms underlying these patterns are associated with inter-subband and intra-subband thermal excitations of electrons. The intra-subband thermal excitations exhibit saturation behavior due to the narrow width of the Landau subband, approximately 2Γ (~ 1 meV). This limits the ability of electrons within this subband to absorb thermal energy.

These characteristics of the electron gas should also manifest in the behavior of other thermodynamic parameters of the system, such as entropy $S(T)$, total energy $U_S(T)$, magnetization $M_S(T)$, and others. In this study, only the chemical potential and electron concentration within the Landau subbands, along with their temperature dependencies, were investigated. For different values of the filling factor ν, graphs depicting the temperature dependence of the chemical potential and electron concentration in the subbands were constructed. The reasons for these dependencies were discussed.

Acknowledgments

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