# THERMODYNAMICS OF SEMICONDUCTIVE FILM WITH A PARABOLIC POTENTIAL IN A STRONG MAGNETIC FIELD

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The expressions for the density of states, magnetic susceptibility, entropy, heat capacity and also for the transverse magnetothermopower of electron gas in a quantum well have been obtained for the cases of nondegenerate statistics and strong degeneracy. It is demonstrated that in the case of strong degeneracy, quantum levels lying below the Fermi level intersect the Fermi level with an increase of the magnetic field, which leads to jumpwise oscillations of theirs magnitude.

## INTRODUCTION

In the past decade, numerous experimental and theoretical investigations have been focused on the variety of thermodynamic and galvanomagnetic properties of semiconductor dots, films and the wires [1-5]. In [1] a linear-response theory was developed for the thermopower of a quantum dot of small capacitance and in the quantum regime of resonant tunneling and at a constant number of electrons on the quantum dot and the oscillations were predicted.

Thermoelectric properties of nanowires in the magnetic field were investigated in [2], where the magnetic splitting of thermopower peaks was predicted and a scheme for measuring of thermopower in a circuit containing a nanowire and leads made from the same material was described. Thermopower peaks are due to the magnetic field on-and-off switching of the energy levels.

The thermoelectric power and longitudinal magneto-Seebeck coefficient of 200 nm diameter single-crystal bismuth nanowire were measured in [3]. It was theoretically calculated that bismuth nanowires should have a high thermoelectric figure of merit over bulk Bi, when the diameter become less than 10 nm. The thermopower and conductance of atomic-size metallic contacts have been studied in [4]. For contacts of atomic dimensions, abrupt steps in the thermopower which coincide with jumps in the conductance were observed.

The electronic conductance in nanowires modeled by soft- and hard-wall confining potentials under the influence of a magnetic field and in the linear and nonlinear rate was investigated in [5]. The behavior of the conductance demonstrates a ``magnetic switch'' (on and off) effect of the quantum electronic transport in nanowires.

It is assumed that a similar behavior should also be observed for thermodynamical parameters of electrons in the quantum well under the conditions of strong degeneracy. This assumption stems from the fact that under these conditions, the dependence of thermodynamical parameters simply reproduces the behavior of the density states at the Fermi level [6].

In the present work the density of states, magnetic susceptibility, entropy, electron heat capacity and magnetothermopower of electrons in a parabolic quantum well are calculated.

At first, the expression for the electron spectrum and the density of states will be given, and then the thermodynamical parameters for the case of nondegenerate statistics and for strong degenerate one will be calculated.

## ELECTRON SPECTRUM IN A PARABOLIC QUANTUM WELL IN A LONGITUDINAL MAGNETIC FIELD

For standard electron dispersion law, the sought spectrum can be represented in the following form [7-10].

$$\varepsilon_{N,k_y,k_z,\sigma} = (N+{}^1/_2)\hbar\omega + \frac{\hbar^2 k_z^2}{2m} + \frac{\omega_0^2}{\omega^2}\frac{\hbar^2 k_y^2}{2m} + \sigma g\mu_B H \qquad (1)$$

Here, the Landau gauge is chosen for the vector-potential $\bar{A}(0, x\cdot H, 0)$; $\omega_0$-characterizes the parabolic potential of the well

$$U = \frac{m\omega_0^2 x^2}{2} \qquad (2)$$

$\omega = \sqrt{\omega_o^2 + \omega_C^2}$, $\omega_c = \dfrac{eH}{mc}$ is the cyclotron frequency, $\mu_B$ is the Bohr magneton, $g$ is the factor of spin splitting, $\sigma = \pm{}^1/_2$, and N is the number of the quantum level.

The coordinate wave function which corresponds to the energy eigenvalue (1), has the form [8,10]

$$\varphi_{N,K_y,K_z}(r) = \varphi_N(x - x_O)e^{ik_y\cdot y + ik_z\cdot z} \qquad (3)$$

where

$$\varphi_N(x - x_o) = \frac{1}{\pi^{1/4}a^{1/2}\sqrt{2^N N!}} e^{-\frac{(x-x_0)^2}{2a^2}} H_N\left(\frac{x - x_O}{a}\right) \qquad (4)$$

$$a = \sqrt{\frac{\hbar}{m\omega}} \qquad (5)$$

$$x_O = -\frac{\omega_c}{\omega}\cdot\frac{\hbar k_y}{m\omega} = -\frac{\omega_c}{\omega}a^2 k_y \qquad (6)$$

$H_N(x)$ - is the Hermite polynomial [11].

The density of states is defined by the expression:

$$\rho(\varepsilon) = \sum_{N,k_y,k_z,\sigma} \delta(\varepsilon_{N,k_y,k_z,s} - \varepsilon) \qquad (7)$$

Then, by moving from the summation over $k_z$ and $k_y$ to the integration and using the expression (6), we obtain

$$\rho(\varepsilon)=\frac{L_y L_Z}{(2\pi)^2}\frac{\sqrt{2m}}{\hbar}\cdot 2\frac{m\omega}{\hbar}\cdot\frac{\omega}{\omega_c}\cdot\sum_{N,s}\int_0^{x_{0m}}\frac{dx_0}{\sqrt{\varepsilon-\varepsilon_{Ns}-bx_0^{2}}} \tag{8}$$

Here,

$$\varepsilon_{Ns}=(N+{}^{1}/_{2})\hbar\omega+sg\mu_B\boldsymbol{H} \tag{9}$$

$$b=\frac{m\omega_0^2}{2\omega_c^2}\cdot\omega^2 \tag{10}$$

Therefore, we have

$$\rho(\varepsilon)=\frac{L_yL_z}{2\pi\hbar^2}\cdot\frac{m\omega}{\omega_0}\cdot\begin{cases}\sum\limits_{N,s}\Theta(-\varepsilon+\varepsilon_{N,s}+b\,{L_x^2}/{4})\cdot\Theta(\varepsilon-\varepsilon_{N,s}) \\ \frac{2}{\pi}\sum\limits_{N,s}\arcsin\sqrt{\frac{b\,{L_x^2}/{4}}{\varepsilon-\varepsilon_{N,s}}}\cdot\Theta\left(\varepsilon-\varepsilon_{N,s}-b\,{L_x^2}/{4}\right)\end{cases} \tag{11}$$

where $L_x$ is the well width and $\Theta(x)$ is the Heaviside function.

## NONDEGENERATE STATISTICS

It is known that the thermodynamical Gibbs potential is determined by the formula

$$\Omega=-k_0T\sum_{N,k_y,k_z,s}ln\left(1+exp\left(\frac{\xi-\varepsilon_{N,k_y,k_z,s}}{k_0T}\right)\right) \tag{12}$$

Entropy

$$S=-\left(\frac{\partial\Omega}{\partial T}\right)_{x,\mathrm{H}} \tag{13}$$

magnetic susceptibility

$$\chi(H,T)=-\frac{1}{VH}\left(\frac{\partial\Omega}{\partial H}\right)_{x,T} \tag{14}$$

heat capacity

$$C_V=S\left(\frac{\partial S}{\partial T}\right)_{V,H} \tag{15}$$

For the nondegenerate statistics,

$$\Omega=-n\cdot k_0\cdot T \tag{16}$$

where

$$n=\frac{mk_0T}{2\pi\hbar^2}\cdot\frac{\omega}{\omega_0}\cdot\frac{ch\left(\frac{g\mu_BH}{2k_0T}\right)}{sh\left(\frac{\hbar\omega}{2k_0T}\right)}\cdot exp(\eta)\cdot erf(t)$$

n is the electron concentration (in our case it is two dimensional concentration), and

$$\chi=\frac{1}{L_xH^2}nk_0T\frac{\omega_c^2}{\omega^2}\left(1+\nu_s\frac{\omega^2}{\omega_c^2}th\nu_s-\nu cth\nu-\frac{2t\,exp\left(-t^2\right)}{\sqrt{\pi}erf(t)\frac{\omega_c^2}{\omega_0^2}}\right) \tag{17}$$

$$S=nk_0\left(2-\eta+\nu cth\nu-\nu_s th\nu_s-\frac{t\,exp\left(-t^2\right)}{\sqrt{\pi}erf(t)}\right) \tag{18}$$

$$C_V=nk_0\left(1+\nu^2\frac{1}{sh^2\nu}+\nu_s\frac{1}{ch^2\nu_s}-\frac{t\,exp\left(-t^2\right)}{\sqrt{\pi}erf(t)}\left(\frac{1}{2}-t-\frac{t\,exp\left(-t^2\right)}{\sqrt{\pi}erf(t)}\right)\right) \tag{19}$$

Here, $$t=\sqrt{\frac{b\cdot L_x^2}{4\cdot k_0\cdot T}} \tag{20}$$

*erf(t)* is the probability integral [11], $k_0$ is the Boltzmann constant.

$$\nu=\frac{\hbar\omega}{2k_0T},\quad \nu_s=\frac{g\mu_BH}{2k_0T},\quad \eta=\frac{\xi}{k_0T} \tag{21}$$

From the Obraztsov's formula for the transverse thermopower [13] follows that,

$$\alpha(H) = -\frac{S}{en} \tag{22}$$

we obtain

$$\alpha = -\frac{k_0}{e}\left(2-\eta+\nu cth\nu-\nu_s th\nu_s-\frac{t\,exp\left(-t^2\right)}{\sqrt{\pi}erf\left(t\right)}\right) \tag{23}$$

In our calculations for GaAs, we used the data from [10] given for the parabolic well with width $L_x=4000Å$, and the height $_1=150meV$, and electron mass $m=0,067m_0$ in order to obtain the estimate $\omega_0=4,437\times10^{12}s^{-1}$. Note that according to Fig.1 in [10], $_1 \quad (m\omega_0^2/2)\times(L_x/2)^2$ in a zero magnetic field.

For InSb semiconductors we assumed that $m=0,016m_0$, and $\hbar\omega_0=7,5meV$ in accordance with [12]. In addition, we put $n=2\times10^{10}cm^{-2}$, and $5\times10^{10}cm^{-2}$ for InSb and GaAs, respectively. The calculated dependences $\chi(H)$ and $C_V(H)$ for InSb, ($g=-51,2$, curve 1) and GaAs ($g=-0,44$, curve 2) at $T=300\ K$ are shown in Fig.1 and Fig.2, respectively.

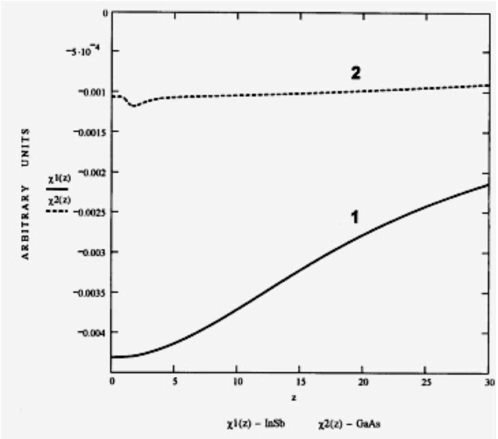


*Fig 1*. The dependence of magnetic susceptibility on the reduced value of the magnetic field $z=w_c(H)/w_0$ for InSb (curve 1) and GaAs (curve 2) for the nondegenerate case.

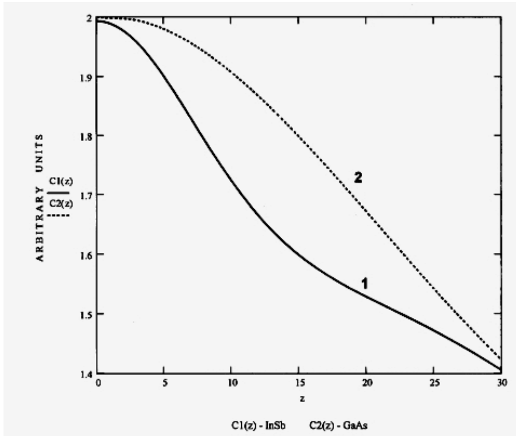


*Fig2*. The dependence of electron heat capacity on the reduced value of the magnetic field $z=w_c(H)/w_0$ for IbSb

## THE CASE OF STRONG DEGENERATION

In the case of strong degeneracy, the magnetic susceptibility, heat capacity and thermopower change nonmonotonously having the oscillatory behavior [3,8].

In the formula given below, it is taken into account that the Fermi level is much lower than $b\times(L_x/2)^2$ at the considered concentrations

$$\chi=\frac{e^2}{2\pi L_x mc^2}\cdot\frac{1}{2\sqrt{1+z^2}}\cdot\sum_{N,s}\left(\eta-s\gamma\frac{m}{2m_0}z-\left(N+\frac{1}{2}\right)\sqrt{1+z^2}\right)\cdot\left(\eta-s\gamma\frac{m}{2m_0}\cdot\frac{2+3z}{z}-3\left(N+\frac{1}{2}\right)\sqrt{1+z^2}\right)\cdot\Phi\left(\eta-s\gamma\frac{m}{2m_0}z-\left(N+\frac{1}{2}\right)\sqrt{1+z^2}\right) \tag{24}$$

$$C_V=\frac{L_yL_zm}{\hbar^2}\cdot\sqrt{1+z^2}\,\frac{\pi}{6}\cdot k_0^2T\cdot\sum_{N,s}\Phi\left(\eta-s\gamma\frac{m}{2m_0}z-\left(N+\frac{1}{2}\right)\sqrt{1+z^2}\right) \tag{25}$$

$$\alpha(H)=-\frac{L_xL_y}{n}\cdot\frac{m\sqrt{1+z^2}}{\hbar}\cdot\frac{\pi}{6}\cdot\frac{k_0^2T}{e}\sum_{N,s}\Phi\left(\eta-s\gamma\frac{m}{2m_0}z-\left(N+\frac{1}{2}\right)\sqrt{1+z^2}\right) \tag{26}$$

where $z=\omega_c/\omega_0$, $\eta=\varepsilon_F/\hbar\omega_0$

Here, the position of the Fermi level is determined from the expression for the concentration and depends weakly on the magnetic field:

$$n = \frac{m\omega_0}{2\pi\hbar}\sqrt{1+z^2}\cdot\sum_{N,s}\left(\eta - \sigma g\frac{m}{2m_0}z - \left(N+\frac{1}{2}\right)\sqrt{1+z^2}\right)\Theta\left(\eta - \sigma g\frac{m}{2m_0}z - \left(N+\frac{1}{2}\right)\sqrt{1+z^2}\right) \qquad (27)$$

As the magnetic field increases, the quantum levels located lower than the Fermi level intersect the Fermi level leading to the abrupt decrease in absolute value of thermopower, magnetic susceptibility and heat capacity. However, between the above abrupt decreases the density of states, the magnetic susceptibility, heat capacity and magnetothermopower increase proportionally to $\omega(H)$ and thus, the oscillatory behavior $\chi(H)$, $C_V(H)$ and $\alpha(H)$ are observed.

The dependences $\chi(H)$, $C_V(H)$ for InSb $n=10^{12}cm^{-2}$ (curve 1) and GaAs $n=5\times10^{11}cm^{-2}$ (curve 2) at T=4,2K are shown in fig.3 and 4, respectively. The concentrations are higher than in the nondegenerate case since our aim was to observe several oscillations.

In the case of InSb, the jumps are nonuniform due to a considerable influence of the quantum level spin splitting.

Thus, in the present paper the magnetic susceptibility, heat capacity and nondissipative transverse magnetothermopower in a quantum well have been investigated. The expressions for the density of states, magnetic susceptibility, entropy, heat capacity and thermopower of electron gas have been obtained. It is shown that in the case of degeneration, the dependence of $\chi(H)$, $C_V(H)$, $\alpha(H)$ on the magnetic field has a nonmonotonous oscillatory behavior.

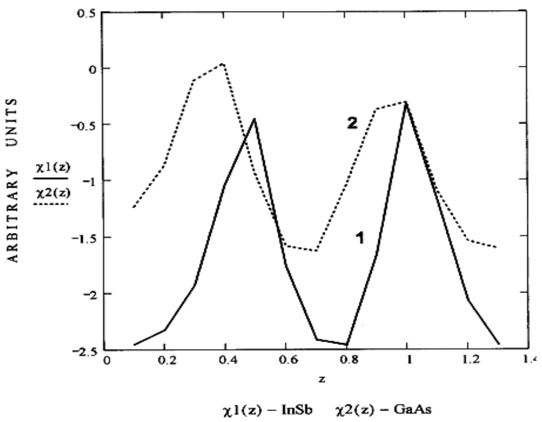


*Fig 3*. The dependence of magnetic susceptibility on the reduced value of the magnetic field $z=\omega_c(H)/\omega_0$ for IbSb (curve 1) and GaAs (curve 2) for the degenerate case.

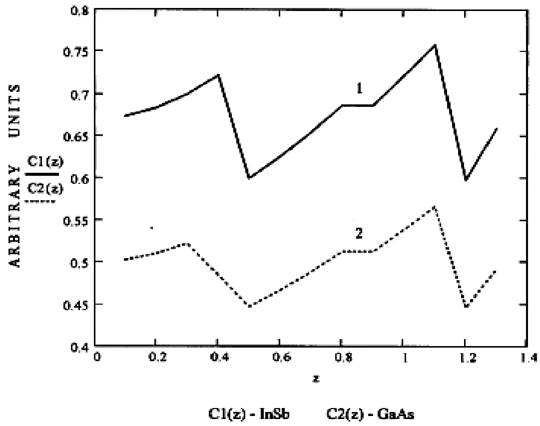


*Fig.4*. The dependence of electron heat capacity on the reduced value of the magnetic field $z=\omega_c(H)/\omega_0$ for IbSb (curve 1) and GaAs (curve 2) for the degenerate case.


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