Influence temperature and strong magnetic field on oscillations of density of energy states in heterostructures with quantum wells Hgcdte/Cdhgte

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Abstract. For the first time, the influence of temperature and a transverse strong magnetic field on the oscillations of the density of energy states is studied in the conduction band of heterostructures with quantum wells HgCdTe/CdHgTe. Analytical expressions are derived for oscillations of the density of states in quantum-dimensional heterostructural materials in the presence of transverse quantizing magnetic fields with a parabolic dispersion law. A new mathematical model has been developed for calculating the temperature dependence of the density of states oscillations in nanosized heterostructural materials under the action of a transverse quantizing magnetic field.

1 Introduction

At present, the interest in applied and fundamental research in the field of condensed matter physics has shifted from bulk materials to nanoscale semiconductor structures. Of particular interest are the properties of the energy spectrum of charge carriers in low-dimensional semiconductor structures under the action of a quantizing magnetic field. Quantizing the energy levels of free electrons and holes in a quantizing magnetic field leads to a significant change in the type of oscillations in the density of energy states in heterostructural materials with quantum wells [1, 2].

In heterostructural materials based on quantum wells, the study of the dependence of the density of energy states on the magnitude of the quantizing magnetic field and occupation provides valuable information on the energy spectra of charge carriers in nanoscale semiconductor structures. When exposed to transverse quantizing magnetic fields in low-dimensional semiconductor materials, the density of states was measured from oscillating dependences of kinetic, dynamic, and thermodynamic quantities - magnetoresistance, magnetic susceptibility, electronic heat capacity, thermoelectric power, Fermi energies, and other physical parameters [3, 4]. From this, it follows that studying oscillations in the density of energy states in the conduction band of a rectangular quantum well in the presence of a transverse and longitudinal magnetic field is one of the urgent problems of modern solid-state physics.

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In particular, in works [5-7] was considered the calculations of the density of states of Landau levels in two-dimensional electron gases are considered for a uniform perpendicular magnetic field and a random field of arbitrary correlation. A semiclassical approach of path integrals has been developed for a random field of arbitrary correlation, and this provides an analytical solution for the density of states of Landau levels. The deviation of the density of states from the Gaussian form increases as the correlation length decreases and the magnetic field weakens [3-5].

Despite the progress achieved in these works, some questions remain open in them, such as the dependence of the density of states on temperature and on a quantizing magnetic field in two-dimensional semiconductor materials and how to determine the temperature dependence of the density of states in a transverse and longitudinal quantizing magnetic field in low-dimensional materials, taking into account thermal smearing.

This work aims to simulate the effect of a transverse quantizing magnetic field and temperature on oscillations of the density of states in heterostructural materials based on quantum wells.

2 Methods

According to the band theory of a solid, the wave function of a free electron, in the presence of an external field, is a solution of the stationary Schrödinger equation with a parabolic dispersion law [8-13]:

$$\left\{-\frac{\hbar^2}{2m^*}\nabla^2+V(r)\right\}\psi(r)=E\psi(r) \tag{1}$$

Here, V(r) is the energy of free electrons in the presence of an external field, E is the energy of charge carriers in the absence of an external field, $\psi(r)$ is the wave function. The dependence of the quantizing magnetic field on the wave function of electrons and the energy spectra of charge carriers in two-dimensional electron gases is determined using Eq. (1), in which the momentum operator should be replaced by the generalized momentum operator in a quantizing magnetic field:

$$\left\{\frac{1}{2m^*}\left(-i\hbar\nabla-eA\right)^2+V(z)\right\}\psi(r)=E\psi(r) \tag{2}$$

Here, A is the vector potential of the induction of a strong magnetic field, $\left[B=rot(A)\right]$. To solve equation (2), the direction of the vector B is chosen in two different ways. In the first case, this vector will be directed along the plane of the two-dimensional layer (along the X-axis) and perpendicular to the Z-axis. For a longitudinal quantizing magnetic field, vector potential A can be chosen in the form of $A=\left(0,-Bz,0\right)$. $\psi_{k\perp m}$ from the Schrödinger equation (2), for a deep rectangular quantum well, takes the following form:

$$\psi_{k\perp m}\left(r\right)=\frac{1}{\sqrt{S}}\exp\left(ik_{\perp}r_{\perp}\right)\varphi_n\left(z-z_0\right) \tag{3}$$

In a quantizing magnetic field, if the width of the quantum well increases, the energy spectrum of free electrons will increase. That is, $a >> \lambda = \sqrt{\frac{\hbar}{eB}}$. Here, a is the width of the quantum well, λ is the magnetic length, which is equal in magnitude to the radius of the characteristic orbit of an electron in a quantizing magnetic field. Hence, the discrete energy levels E_n will be equal to the energies of the harmonic quantum oscillator:

$$E_N = \hbar\omega_c\left(N + \frac{1}{2}\right), \ N = 0,1,2,3.... \quad (4)$$

Where, $\hbar\omega_c\left(N + \frac{1}{2}\right)$ is the energy of motion of a free electron in the XZ plane, these energies are called discrete Landau levels.

In three-dimensional and two-dimensional electron gases, a change in the energy spectrum of charge carriers leads to a change in the oscillation of the density of states in a quantizing magnetic field. In works [14, 15], an analytical expression was derived for oscillating the density of states in three-dimensional electron gases in the presence of a quantizing magnetic field with a nonparabolic dispersion law. The temperature dependence of the oscillations of the density of energy states in a strong transverse magnetic field was discussed there.

Now, consider the dependence of the oscillations of the density of states on the transverse quantizing magnetic field in a rectangular quantum well or two-dimensional electron gases. In this case, the magnetic field is directed along the Z axis and will be perpendicular to the XY plane. Here, the energies of free electrons are quantized (discretely) along the Z axis, and charge carriers move freely.

Can select the vector potential of the magnetic induction in the form of $A = \left(0, Bx, 0\right)$. Hence, by solving equation (1), instead of formula (3), we can obtain the following function:

$$\psi_{Ky\,Nm}\left(r\right) = f_N\left(x - x_0\right)\varphi_m\left(z\right) \quad (5)$$

Here, $\varphi_m\left(z\right) = \begin{cases} \sqrt{\frac{2}{a}}\cos\left(m\frac{\pi}{a}z\right), \ m = 2n+1 \\ \sqrt{\frac{2}{a}}\sin\left(m\frac{\pi}{a}z\right), \ m = 2n \end{cases}$ is the envelope function of the dimensional quantization levels of the quantum well [12]. $f_N\left(x - x_0\right)$ is a solution to the Schrödinger equation with zero boundary conditions for a quantum harmonic oscillator. In the same solution, the equation takes the following form:

$$\left\{-\frac{\hbar^2}{2m^*}\frac{d^2}{dx^2} + \frac{1}{2}m^*\omega_c^2(x - x_0)^2\right\}f_N(x - x_0) = E_N f_N(x - x_0) \quad (6)$$

Here, $x_0 = -\frac{\hbar k_y}{eB}$. The eigenvalues of the energies $E_N$are called discrete Landau levels, corresponding to the functions from (5). In a deep rectangular quantum well, the discrete energy spectrum of dimensional quantization is:

$$E_m = \frac{\pi^2 \hbar^2}{2md^2} m^2, \quad m = 1, 2, ... \tag{7}$$

Hence, taking into account formulas (4) and (7), the energy eigenvalue $E_{Nm}$is determined by the following formula:

$$E_{Nm} = \hbar \omega_c \left(N + \frac{1}{2} \right) + \frac{\pi^2 \hbar^2}{2m^* d^2} m^2 \tag{8}$$

As can be seen from the formula, the motion of free charge carriers in all three directions is limited, and in a transverse quantizing magnetic field, the quantum well becomes an analog of a quantum dot. In addition, the energy spectrum of free electrons will be completely discrete; each level in it is characterized by two quantum numbers: N_L ($N = N_L$ is the number of Landau levels) and N_Z ($m = N_Z$ is the number of quanta in the Z axis). Then, for a transverse quantizing magnetic field in two-dimensional electron gases, the oscillation of the density of states, normalized to a unit area, has the form of a sum of delta functions:

$$N_{S,Z}^{2d}(E, B) = \frac{eB}{\pi \hbar} \sum_{N_L, N_Z}^{\infty} \delta\left(E - E\left(N_L, N_Z\right)\right) \tag{9}$$

Thus, in the presence of a transverse quantizing magnetic field corresponding to formula (9), it is possible to calculate the oscillations of the density of states heterostructures with quantum wells. But, both formulas do not consider thermal smearing in discrete Landau levels.

Effect of Temperature and a Transverse Strong Magnetic Field on Oscillations of the Density of Energy States in Heterostructures with Quantum Wells.

Let us now consider the temperature dependence of the oscillations of the density of states in low-dimensional solids under the action of a transverse quantizing magnetic field. As is known, the effect of temperature on the Landau levels can be described by expanding the oscillations of the density of energy states into a series in terms of delta-shaped functions [14-16]. The study of the oscillations of the density of energy states using the series expansion in terms of delta-shaped functions made it possible to explain the temperature dependence of discrete Landau levels in two-dimensional semiconductor materials. The temperature dependence of the oscillations of the density of states is determined by the thermal smearing of discrete Landau levels in a quantizing magnetic field. At absolute zero temperature, the Gaussian distribution functions are delta-shaped and are defined by the following expression [16, 17]:

$$Gauss(E, T) = \frac{1}{kT} \cdot \exp\left(-\frac{\left(E - E_i\right)^2}{\left(kT\right)^2} \right) \tag{10}$$

Then, thermal smearing can be described by the temperature dependence of the Gaussian distribution function. The thermal smearing of discrete Landau levels with energy $E\left(N_L, N_Z\right)$ is determined by the Shockley-Reed-Hall statistics [15-17]. Formula (9) does not consider the thermal smearing of discrete Landau levels. If $N_{S,Z}^{2d}\left(E,B,T,d\right)$ is expanded into a series in terms of Gaussian functions, then the temperature dependence of the oscillations of the density of energy states in two-dimensional electron gases can be considered. In this way, one can obtain the temperature dependence of the oscillations of the density of states in a transverse quantizing magnetic field. At low temperatures, the Gaussian distribution functions turn into a delta-like function of the form:

$$\underset{T\to 0}{Gauss}\left(E,E_i,T\right)\to\delta\left(E-E_i\right) \tag{11}$$

Thus, with the help of formulas (8), (9), (10), and (11), we obtain the following analytical expressions:

$$N_{S,Z}^{2d}\left(E,B,T,d\right)=\sum_{N_L,N_Z}^{\infty}\frac{eB}{\pi\hbar}\cdot\frac{1}{kT}\cdot\exp\left(-\frac{\left(E-\left(\hbar\omega_c\left(N_L+\frac{1}{2}\right)+\frac{\pi^2\hbar^2}{2m^*d^2}N_Z^2\right)\right)^2}{\left(kT\right)^2}\right) \tag{12}$$

Here, $N_{S,Z}^{2d}\left(E,B,T,d\right)$ is oscillations of the density of energy states for an infinitely deep rectangular quantum well; d is the thickness of the quantum well; N_L is the number of Landau levels for a rectangular quantum well; N_Z is the number of quanta along the Z axis; B is the induction of the transverse quantizing magnetic field.

This formula is the temperature dependence of the oscillation of the density of energy states in two-dimensional semiconductor materials when exposed to a transverse quantizing magnetic field. The obtained expression is convenient for processing experimental data on oscillations of the density of energy states in two-dimensional electron gases at different temperatures and in transverse magnetic fields. Thus, a mathematical model has been obtained that describes the temperature dependence of the oscillations of the density of states in nanoscale semiconductor structures.

3 Results and discussion

Now, for specific nanoscale semiconductor materials, we analyze the temperature dependence of the oscillations of the density of states in a transverse quantizing magnetic field. In work [18], the energy spectra of cyclotron resonance of free electrons in asymmetric heterostructures with HgCdTe/CdHgTe quantum wells were determined in a quantizing magnetic field. Here, the thickness of the $Cd_xHg_{1-x}Te$ quantum well is d=15 nm, the magnetic field is B=15 T, and the temperature is T=4.2 K. These papers did not discuss the temperature dependences of the density of states $N_{S,Z}^{2d}\left(E,B,T,d\right)$ for these materials. Figure 1 shows the oscillations of the density of energy states for the quantum well $Cd_xHg_{1-x}Te$ d=15 nm [18] at T=4.2 K and with a transverse quantizing magnetic field B=15 T. There $N_{S,Z}^{2d}\left(E,B,T,d\right)$ is calculated using formula (12).

In Figure 1, the number of discrete energy levels is ten. These discrete energy peaks are called Landau levels (N_L=10), which are observed in the conduction band. It shows oscillations of the density of energy states in a quantizing magnetic field $\hbar\omega_c = 0,02\ eV$ at T=4.2 K, kT=4.10-4 eV, $\frac{\hbar\omega_c}{kT} = 50,\ kT << \hbar\omega_c$. In this case, the thermal smearing of the Landau levels is very weak, and the oscillations in the density of energy states do not feel a deviation from the ideal shape. The first discrete Landau level (N_L=0) appeared at the bottom of the conduction band of the quantum well. The second (N_L=1), third (N_L=2), and other discrete Landau levels are located above the bottom of the conduction band of the quantum well. This way, one can calculate the Landau level peaks in the quantum well valence band at low temperatures. Figure 2 are shown temperatures of 4.2 K, 20 K, 40 K, 60 K, 80 K, and 100K. It can be seen from Figure 2 that with increasing temperature, the sharp peaks of Landau levels begin to smooth out, and at sufficiently high temperatures, discrete energy densities of states turn into continuous energy spectra. These results were obtained for a constant quantum well thickness and magnetic field. Using formula (12), one can calculate the dependence of the quantum well thickness on the oscillation of the density of energy states with a parabolic dispersion law.

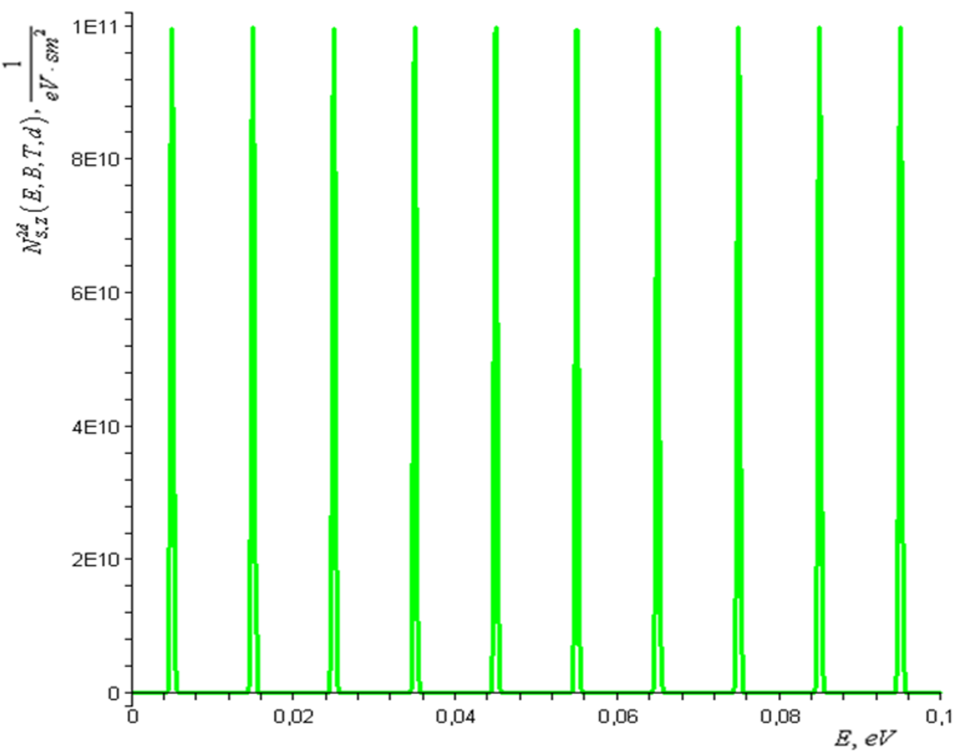

Fig. 1. Oscillations of density of energy states in heterostructures with quantum wells HgCdTe/CdHgTe($Cd_xHg_{1-x}Te$ quantum well, d=15 nm [18]) at B=15 T and T=4.2K. Calculated by formula (12).

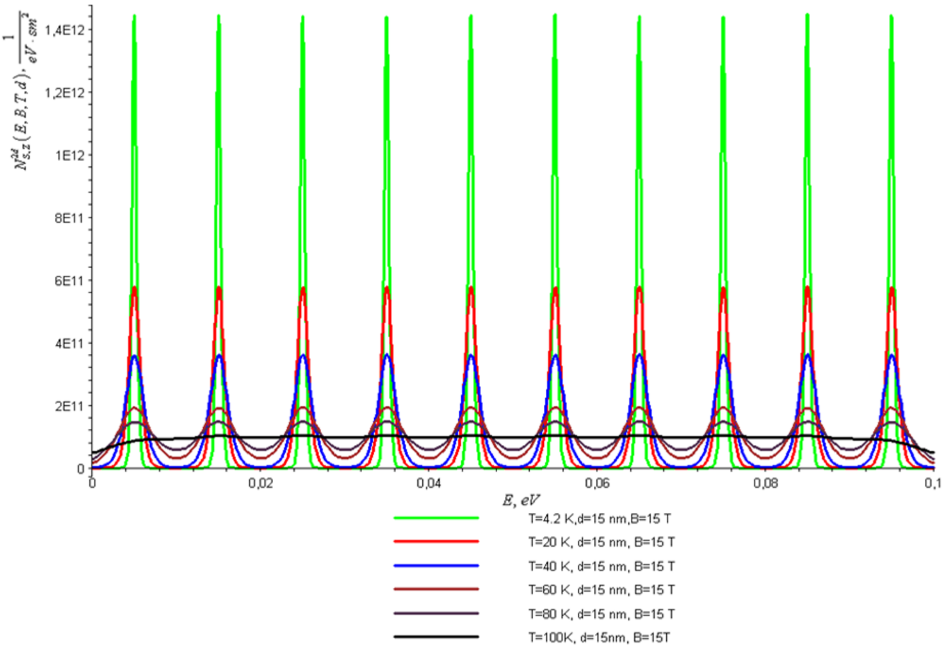

Fig. 2. Effect of temperature and a transverse strong magnetic field on oscillations of density of energy states in heterostructures with quantum wells HgCdTe/CdHgTe calculated by formula (12).

4 Conclusion

Based on the study, the following conclusions can be drawn: Analytical expressions for oscillations of the density of states in heterostructural materials with quantum wells in the presence of transverse quantizing magnetic fields are derived. A new mathematical model has been developed to determine the temperature dependence of the oscillations in the density of energy states in two-dimensional semiconductor materials in the presence of a transverse quantizing magnetic field. It is shown that with increasing temperature, the discrete Landau levels are smoothed out due to thermal smearing, and oscillations in the density of energy states are not observed in heterostructural materials with quantum wells. The proposed mathematical model makes it possible to calculate the high-temperature density of states for the HgCdTe/CdHgTequantum well. It is shown that the discrete Landau levels in the HgCdTe/CdHgTe quantum well, measured at T=4.2 K, transform into a continuous energy-state density spectrum at high temperatures (T=100 K).

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