

Modeling of Landau levels, Hall and longitudinal resistance in the topological Anderson insulator based on HgTe/Hg_{0.3}Cd_{0.7}Te quantum well

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The Landau levels, the conditions of the Hall resistance quantization and the behavior of the longitudinal resistance of the edge states in the magnetic field are studied for the HgTe/Hg_{0.3}Cd_{0.7}Te quantum well with (013) orientation and 14.1 nm width, corresponding to the semi-metallic spectrum and near the charge neutrality point. Based on recent experiments for such structure with a disorder in the phase of a topological Anderson insulator and applying the localization theory for the edge states in a magnetic field, the modeling of the observation threshold of the Hall conductance plateau is performed, as well as of the dependence of the longitudinal resistance of the edge states, at different temperature. The modeling results are in a good agreement with the experimental data.

Keywords: topological Anderson insulator, semimetal, edge states, localization, Hall resistance, longitudinal resistance.

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1. Introduction

Topological insulators (TI) based on quantum wells (QW) HgTe/Hg_{1-x}Cd_xTe represent one of the first and deeply studied examples of this intensively studied phase of matter [1,2]. One of the attributes of this phase is the localized nature of the bulk states, in the zone of which the Fermi level is located, along with the presence of delocalized edge states. Localization of states in a volume at the Fermi level can occur both due to its location in the band gap and due to disorder that localizes initially propagating bulk states. In the latter case, when forming delocalized edge states, one speaks of a topological Anderson insulator (TAI) [3–5].

The presence of a gap in the spectrum of bulk states between the valence band and the conduction band is an attribute of „classical“ TI. Meanwhile, a semimetallic spectrum appears at a certain crystallographic orientation and well thickness in the quantum wells of HgTe/Hg_{1-x}Cd_xTe, in which the conduction band overlaps by several meV with the valence band [6,7]. Near the point of charge neutrality, near which the position of the Fermi level can change, there are two types of carriers in the system - electrons and holes. If a sufficiently strong disorder appears in such a structure, then as the temperature decreases, holes are localized first, and then electrons. At the same time, as experiments show [8], there are signs of the existence of edge states through which the main transport proceeds at low temperatures, when bulk states are localized due to disorder.

Results demonstrating the behavior of longitudinal and Hall conductivity in a magnetic field with induction up to 1.5 T were obtained in recent experiments [9], for a structure based on the HgTe/Hg_{0.3}Cd_{0.7}Te quantum well with an orientation (013) and a thickness of 14 nm characterized by strong disorder. It was found that in a weak magnetic field, the sample behaves like a two-dimensional topological insulator with a weakly magnetic-field-dependent longitudinal resistance detected in both local and non-local geometries. In this case, the Hall resistance depends on temperature and has different values. Then, a strong increase of longitudinal resistance begins after reaching a relatively weak threshold field of $B_0 \sim 5$ mT, which increases at low temperature $T = 0.1$ K by 2 orders in the field of $B_1 \sim 0.1$ T. At the same time, the Hall resistance shows strong fluctuations. This behavior was classified in Ref. [9] as the phase of the Anderson insulator, when edge states experience localization. Finally, the character of the resistances changes again when the magnetic field reaches the value of $B_c \sim 0.4$ T: the longitudinal resistance begins to decrease strongly (by 2–3 orders of magnitude), and the Hall resistance reaches a plateau h/e^2 , weakly dependent on temperature. It was concluded in Ref. [9] that this regime corresponds to the quantum Hall effect (QHE) phase with a Landau level filling factor of $\nu = 1$. It is of great interest to find out how the characteristic threshold values of the magnetic field B_0 and B_c are determined, and also to build a quantitative picture of the dependence of the longitudinal and Hall resistances on the magnetic field.

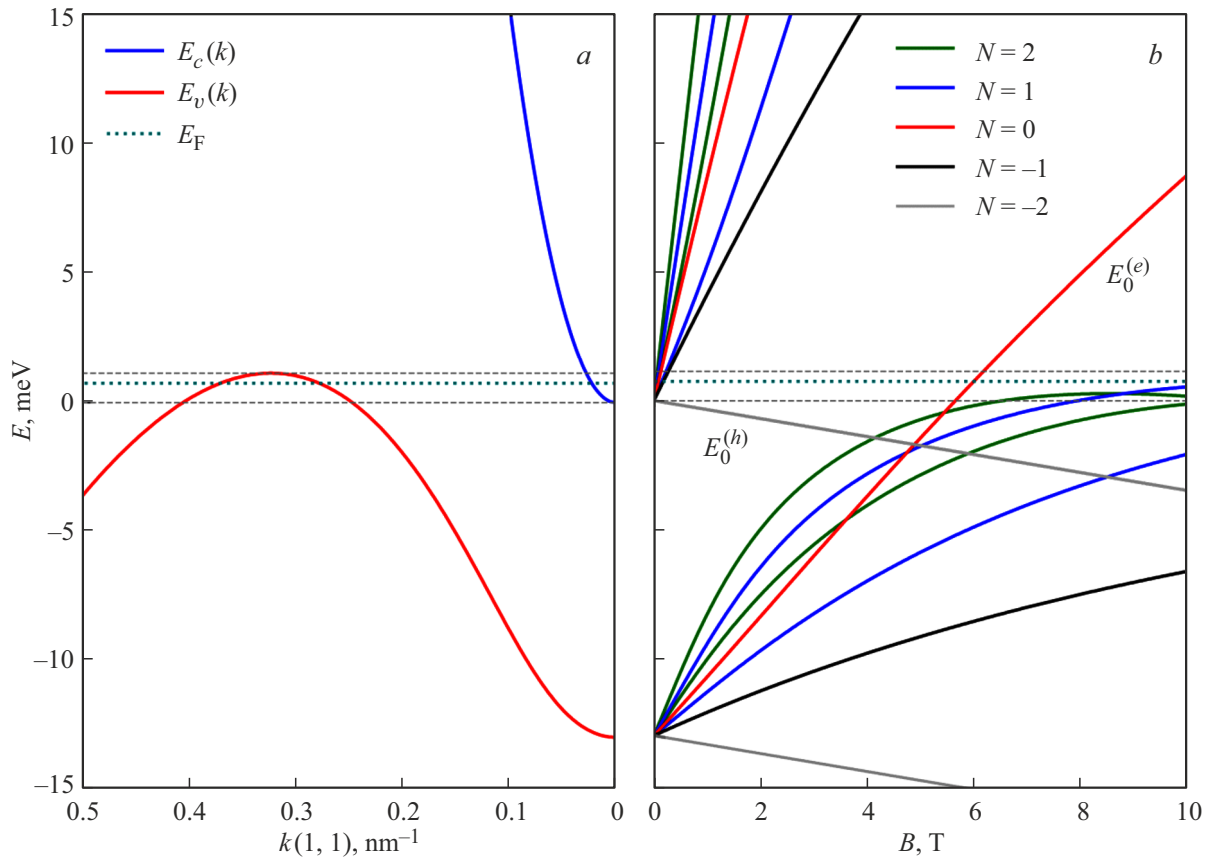


Figure 1. *a* is the spectrum in the quantum well HgTe/Hg_{0.3}Cd_{0.7}Te along the direction (1,1) at $k_x = k_y$. The area of overlap of the electronic $E_c(k)$ and hole $E_v(k)$ bands is bounded by dotted lines, E_F shows the Fermi level; *b* is the structure of the Landau levels with the wave function index N , where the levels $E_0^{(e)}$ and $E_0^{(h)}$ with linear dispersion law are highlighted.

In this paper, we will try to answer some of the questions raised in Ref. [9] by constructing model estimates of the results obtained in it. We will use the results of the theory of the quantum Hall effect in the presence of disorder [10] and the theory of localization of edge states in the presence of a magnetic field [11]. Sec. 2 will consider the structure of the Landau levels in the system under consideration and the quantization of the Hall resistance in the presence of disorder. Sec. 3 will discuss modeling the behavior of longitudinal conduction in a magnetic field. The conclusions of the work are presented in sec. 4.

2. Modeling of Landau levels and quantization of Hall conductivity

Our first task is to model the Landau levels for a two-dimensional spectrum in an HgTe/Hg_{0.3}Cd_{0.7}Te quantum well with orientation (013) and thickness of 14 nm. The band structure of the system of interest in the absence of a magnetic field was calculated in Ref. [6]. Methods for calculating the spectrum in the framework of the 8-band Kane model, including in the magnetic field, are described in a number of papers (see, for example, [12–17]). The final

result of this calculation is shown in Figure 1, where the panel *a* shows the spectrum along the direction $k_x = k_y$ of the two-dimensional Brillouin zone. There is an overlap of the electron and hole bands on the scale of ~ 3 meV, which corresponds to the semimetal structure [6]. The overlap area is highlighted with dotted lines in Figure 1, *a*. If the Fermi level is near the point of charge neutrality, as in the experiments in Ref. [9], then it also lies inside this region. The Landau levels in the magnetic field perpendicular to the plane of the well are shown in Figure 1, *b*, where the indexes N mark the states of the column vector constructed from Landau levels with different numbers [12–15]. As is known, in a system with interacting bands, the Landau levels exhibit a nonlinear dependence on the magnetic field, with the exception of two „zero“ levels $E_0^{(e)}$ and $E_0^{(h)}$ [12–17]. These two levels have a linear law of dispersion in the absence of terms in the Hamiltonian responsible for mixing the states of heavy and light holes due to the presence of the [16,17] interface, which we do not take into account in our model. The level $E_0^{(e)}$, corresponding to the electronic basic function, begins from the area of overlap of the energy band lying below, which is caused by the inversion of the spectrum in this structure.

Let's discuss the contribution of the Landau levels in Figure 1, *b* in quantization of Hall conductivity. The formation of the Hall plateau was observed in the field starting from $B_c \sim 0.4$ T in experiments in Ref. [9]. The contribution to the Hall resistance is given by the electronic level $E_0^{(e)}$, related to the „zero“ levels linear in the magnetic field in such a field as follows from Figure 1, *b*, at the position of the Fermi level near the point of charge neutrality, i.e., near the middle of the region of overlap of the electron and hole bands. It remains below the Fermi level in fields up to 6 T, which ensures the formation of a Hall step with a fill factor of $\nu = 1$, when the Hall resistance reaches the value of $R_H = h/(\nu e^2)$ with $\nu = 1$, which was observed in experiments [9]. As for the hole levels, there is only one level $E_0^{(h)}$ located below the Fermi level on the side of the filled states for holes, which also belongs to the „zero levels“, as can be seen in Figure 1, *b*. It crosses the Fermi level already in a weak magnetic field ~ 0.1 T and does not contribute to the Hall resistance in stronger fields.

The question arises — why is the contribution of the hole level $E_0^{(h)}$ in the Hall resistance in the experiment in Ref. [9] not traced in the fields below $B_c \sim 0.4$ T. To answer this question, we will use the result of the theory of the quantum Hall effect in the presence of disorder [10]. According to it, monitoring of the QHE state is possible if the condition is met

$$\omega_c \tau > 1, \quad (1)$$

where the cyclotron frequency

$$\omega_c = eB/m^*c \quad (2)$$

depends on the effective mass of m^* , and τ is a lifetime between the acts of elastic scattering. The condition (1) is equivalent to the condition

$$\hbar\omega_c > \hbar/\tau, \quad (3)$$

which means that the distance between the centers of the Landau levels must exceed their broadening \hbar/τ . Let us use the results of experiments in Ref. [9] to assess the broadening of Landau levels due to disorder. It is possible to estimate the magnitude of this broadening in terms of the activation energy V_a , experimentally determined using the temperature dependence of resistance in a zero magnetic field $R = R_0 \exp(V_a/2kT)$ [9]. We obtain from this that

$$\hbar/\tau \sim V_a = 1.7 \text{ meV}. \quad (4)$$

According to (4), the lifetime is

$$\tau \sim 3.6 \cdot 10^{-13} \text{ c}. \quad (5)$$

Effective masses of electrons and holes, according to experimental results [6], are in the range of $(0.02-0.03)m_0$ for electrons and $(0.2-0.3)m_0$ for holes. Choosing the value $0.025m_0$ for electrons and estimating the lifetime according

to (5), we obtain from (1) that the observation of the QHE regime for electrons is possible in the fields

$$B > B_c, \quad (6)$$

where $B_c = 0.39$ T. The experimental results in Ref. [9] indicate that the transition from the insulator mode to the QHE mode occurs under a magnetic field satisfying condition (6).

The reasoning given above makes it possible to explain the absence of a hole contribution to the Hall resistance. According to (1)–(6), holes will begin to contribute to the magnetic field starting from $B_c(h) \sim 3.9$ T, since their effective mass is an order of magnitude greater than the mass of electrons [6]. These considerations are in line with the statements in the papers in Refs. [8,9], according to which holes are localized before electrons. The experiments in Ref. [9] were limited by the magnitude of the magnetic field in 1.5 T, so the contribution of holes to the Hall resistance was not observed.

3. Calculation of longitudinal resistance in a magnetic field

The behavior of longitudinal resistance as a function of the magnetic field in samples of similar geometry to samples from the experiments we are interested in [9], but in a well with a thickness of 8.3 nm, was experimentally studied in Ref. [18]. There, a decrease in longitudinal conductivity was detected both with a decrease in temperature and with an increase in the magnetic field. An activation formula has been proposed for the dependence of conductivity on the magnetic field and temperature

$$G \sim \exp(-\Delta_b/kT). \quad (7)$$

The magnetic field-dependent activation energy Δ_b is based on Figure 2, *d–e* in Ref. [18]. In terms of its physical meaning, it corresponds to a gap in the spectrum of edge states, which is calculated, for example, in Ref. [17]. We want to use an expression like (7) to calculate the dependence of the local resistance R_{loc} in the discussed experimental study [9]. The mechanisms of localization of edge states in a magnetic field have been discussed in a number of papers (see, for example, in Refs. [11,13,16]). We will use some results from Ref. [11], where the scattering processes on the disorder potential are considered in conjunction with the electron-electron interaction.

— In two-dimensional topological insulators with disorder, there is a threshold magnetic field B_0 , below which the longitudinal resistance of the sample is determined by the localization length independent of the magnetic field l_u , determined by the disorder potential and depending on the length of the conducting segment according to the formula

$$R(L) = R_0 \exp(L/l_u), \quad (8)$$

where R_0 has a value of the order of the resistance quantum h/e^2 .

– When the magnetic field exceeds the threshold value of B_0 , the resistance will depend on the localization length of l_b in the magnetic field according to the same law (8) with replacing l_u with l_b , while the localization length depends on the magnetic field according to the formula

$$l_b = \hbar v / \Delta_b, \quad (9)$$

where v is the characteristic group velocity of edge states, Δ_b is the gap that opens in the spectrum of edge states, i.e., the activation energy mentioned above in (7). The transition occurs in a magnetic field B_0 , in which the localization length l_b in (9) equates with the localization length l_u of the disorder potential. With a further increase in the magnetic field, the length l_b in (9) continues to decrease, and localization occurs on its scale as on the smallest of the two (l_u, l_b). Typical dependence of l_b on the magnetic field, according to Ref. [11], has the form

$$l_b \sim B^{-2/(3-2K)}, \quad (10)$$

where the Luttinger parameter K determines the strength of the electron-electron interaction and the associated scattering processes, including in the presence of a disorder potential. The limit $K \rightarrow 0$ corresponds to a strong interaction when the formula (10) gives the dependence $l_b \sim B^{-2/3}$.

We estimate the localization length l_u as a function of the disorder potential, i.e., in a zero magnetic field, as follows. According to the experimental data presented in Ref. [9], at low temperatures the local resistance reaches a value of 10^6 Ohms. This means that the resistance increases by 2 orders of magnitude in comparison with the quantum of resistance of $r_0 = h/e^2 = 26$ kOhm, i.e., according to (8), the parameter

$$x = \ln(R/R_0) = L/l_u \quad (11)$$

is equal to $\ln(10^2) \sim 4.61$. The characteristic length L of the conducting segment in Ref. [9], on which the local resistance R_{loc} is measured, was $L \sim 100 \mu\text{m}$. This means that, according to (11), the localization length of edge states due to disorder can be estimated as

$$l_u \sim 20 \mu\text{m}. \quad (12)$$

This value significantly exceeds the localization length estimates for bulk states with a characteristic lifetime (5).

The estimate of (12) allows determining the threshold magnetic field at which the length of localization in the magnetic field (10) equates with (12). To do this, we will use experimental data from Ref. [18] for the size of gap Δ_b . The dependence Δ_b is nonlinear in fields exceeding 25 mT. We approximate it as follows for obtaining the best agreement with the experimental data in Ref. [18]:

$$\Delta_b(B) = \Delta_0((1 + B/B_0)^{2/3} + c), \quad (13)$$

where $\Delta_0 = 10 \mu\text{eV}$ and $B_0 = 5$ mT, and constant $c = 1 - 2^{2/3}$. The values Δ_0 and B_0 are selected from the

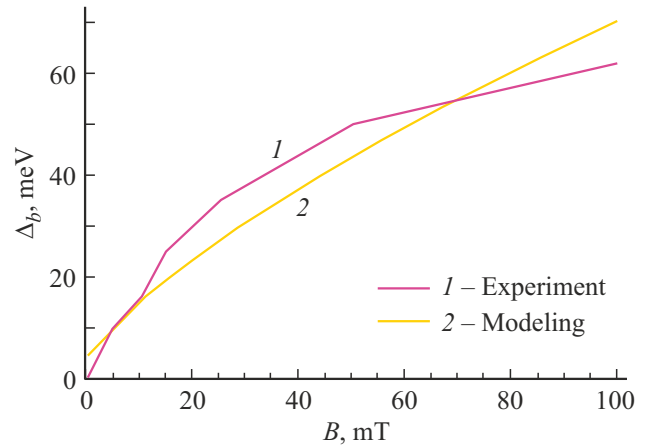


Figure 2. Experimental results for the gap in the spectrum Δ_b obtained in Ref. [18] (1) together with simulation results using the formula (13) (2).

condition that the value $\Delta_b = \Delta_0$ in the field B_0 is such that the localization length (9) in the magnetic field will be equal to the localization length (12) due to the disorder. The graph of the function (13) is shown in Figure 2 by the orange curve 1, next to which a pink polyline 2 connects points based on experimental data from Ref. [18]. Figure 2 shows that there is a fairly good agreement with the experiment in the range of magnetic fields from 0 to 100 mT, for which experimental results were obtained in Ref. [18].

It should be noted that the approximation (13) in accordance with (9) leads to a dependence of the localization length on the magnetic field in the form $l_b \sim B^{-2/3}$, which according to the general theory [11], from which the formula (10) follows, means a strong electron-electron interaction in the limit $K \rightarrow 0$.

Let's move on to calculating the local resistance R_{loc} . First, we calculate the local resistance at different temperatures using a formula close to (7). Experimental results in Ref. [9] suggest that resistance depends exponentially on the ratio Δ_0/kT which power index is smaller than unity. It is most satisfactorily obtained to approximate the experimental results by dependence

$$R(T, B < B_0) = R_0 \exp((\Delta_0/kT)^{1/2}), \quad (14)$$

where the value $R_0 \sim 10^5$ Ohms, i.e. exceeds the quantum of resistance r_0 by ~ 4 times. The formula (14) can be applied in weak magnetic fields $B < B_0$, where $B_0 = 5$ mT, when localization is determined by a length (12) independent of the magnetic field. The graphs of the function (14), constructed for the temperature $T = 2, 1, 0.5, 0.2, 0.1$ K, are shown in the left part of Figure 3 with horizontal lines drawn up to the value $B = B_0$. This region corresponds to a topological insulator with disorder, i.e., a topological Anderson insulator.

Starting with the magnetic field $B = B_0$, we use an approximation of the same type as (14), but in which the

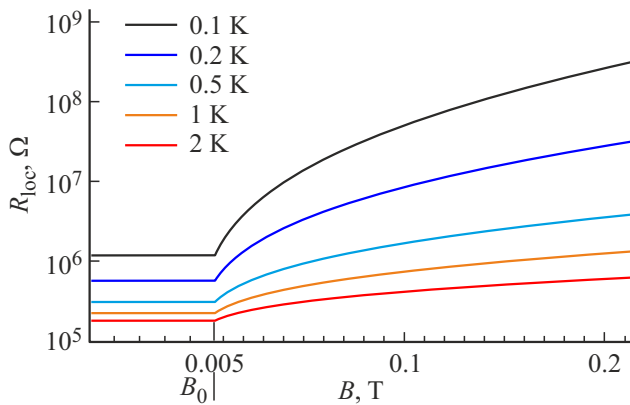


Figure 3. Simulation of longitudinal (local) resistance R_{loc} for experiments [9], executed according to (14) and (15). Different curves correspond to different temperatures. The area to the left of the threshold field $B_0 = 5$ mT corresponds to a topological insulator with fixed localization length l_u of edge states, the area to the right of B_0 corresponds to a decreasing one according to (10) with index $K = 0$ the length of localization in the magnetic field.

gap in the spectrum $\Delta_b(B)$, or activation energy, is no longer equal to Δ_0 , but it depends on the magnetic field and is approximated by the formula (13). The resistance in this mode is

$$R(T, B > B_0) = R_0 \exp((\Delta_b(B)/kT)^{1/2}). \quad (15)$$

Graphs of the function (15), constructed for the same set of temperature values, $T = 2, 1, 0.5, 0.2, 0.1$ K, are plotted in the right part of Figure 3. This is the insulator mode, in which the localization length of the edge states decreases with an increase in the magnetic field. It should be noted that the modes (14) and (15) correspond physically to the same system, since the edge states continue to exist, but with the transition from (14) to (15), the length of their localization becomes variable, decreasing with increasing magnetic field. Therefore, in our opinion, the transition from a topological insulator to the usual resistance behavior in Figure 3 should be considered quantitative, but not qualitative. In general, the agreement of the results in Figure 3 with experimental data from Ref. [9] in fields up to ~ 300 mT can be considered satisfactory.

The value $B_2 = 200$ mT, is selected as the right boundary of the magnetic field interval in Figure 3. According to experimental data from Ref. [9], at values of $B > B_2$, a decrease in local and nonlocal resistances is observed due to the transition to the quantum Hall effect mode described in sec. 2 in this paper. In the field $B_c \sim 390$ mT, according to (6), conditions for observing QHE are already being created for bulk states that remained localized and did not participate in transport at low temperatures. Therefore, our approximations in fields of order and higher than B_2 lose their validity, as the transport of edge states with increasing resistance begins to transform into transport of bulk and edge states in the quantum Hall effect mode. A detailed

calculation of these transient modes and the microscopic structure of edge states in a magnetic field is an interesting task for future studies.

4. Conclusion

The spectrum and Landau levels have been modeled for states in the HgTe/Hg_{0.3}Cd_{0.7}Te quantum well with orientation (013) and thickness of 14 nm in the phase of a topological Anderson insulator with strong disorder for the purpose of constructing theoretical estimates of recent experiments in Ref. [9] for transport. It is shown that the quantization threshold of the Hall resistance, which is manifested when the cyclotron frequency exceeds the magnitude of the broadening of the Landau levels due to disorder, corresponds to experimental data. A model of the dependence of the longitudinal resistance on the magnetic field for transport through edge states is constructed, taking into account the gap in the spectrum due to disorder, which turns into a gap that grows with the magnetic field according to experimental data. The obtained dependences of resistance on the magnetic field for different temperatures are in good agreement with the experimental results. To build a detailed picture of the edge states in a topological Anderson insulator in a magnetic field, it is assumed that research will continue in the future, primarily focusing on the construction of microscopic models.

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Conflict of interest

The authors declare no conflict of interest.

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