

doi:

O.E. RAICHEV

V.E. Lashkaryov Institute of Semiconductor Physics, Nat. Acad. of Sci. of Ukraine  
(41, Prosp. Nauky, Kyiv 03680, Ukraine; e-mail: raichev@isp.kiev.ua)

## EFFECTIVE HAMILTONIAN AND DYNAMICS OF EDGE STATES IN TWO-DIMENSIONAL TOPOLOGICAL INSULATORS UNDER MAGNETIC FIELDS

UDC 539

*The magnetic field opens a gap in the edge state spectrum of two-dimensional topological insulators, thereby destroying the protection of these states against backscattering. To relate properties of this gap to parameters of the system and to study the dynamics of electrons in edge states in the presence of inhomogeneous potentials, the effective Hamiltonian theory is developed. Using this analytical theory, the quantum-mechanical problems of edge-state electron transmission through potential steps and barriers and of motion in a constant electric field are considered. The influence of a magnetic field on the resistance of two-dimensional topological insulators based on HgTe quantum wells is discussed together with comparison to experimental data.*

*Keywords:* topological insulators, HgTe quantum wells, edge states, energy gap.

### 1. Introduction

The two-dimensional (2D) topological insulators (also known as quantum spin Hall states) experimentally realized in HgTe-based quantum wells [1–5] represent a unique state of matter characterized by the existence of a pair of helical counter-propagating one-dimensional (1D) conducting channels at the edges of a 2D system. These edge states have gapless energy spectrum and are topologically protected due to the time reversal symmetry, which means that electrons in these states move without backscattering, if the inelastic scattering is neglected. When the Fermi energy stays in the bulk insulating gap, the edge states determine the electron transport. The resistance quantization observed [1] at low temperatures in the HgTe quantum well samples of macroscopic (1  $\mu\text{m}$ ) length and subsequently confirmed in nonlocal resistance measurements [4] is a convincing proof for the ballistic transport of electrons in the edge states.

The problem of influence of magnetic fields on the transport properties of 2D topological insulators has appeared immediately after the discovery of these systems. Experimentally, it was found [1–3] that the field perpendicular to the quantum well plane,  $B_z$ , considerably suppresses the conductance already at  $B_z \sim 0.01$  T, while the in-plane magnetic field suppresses the conductance only when it is strong enough, of the order of 1 T. It was also established that the conductance depends on the direction of the magnetic field in the quantum well plane [3]. Later on, it was demonstrated [6, 7] that similar phenomena also take place in long samples, where the edge-state transport is not ballistic and the resistance is much larger than the resistance quantum. However, the effect of a perpendicular magnetic field under these conditions is much smaller and manifests itself at  $B_z \sim 1$  T, similar to the case of in-plane field. To describe the effect of a perpendicular field, several theoretical approaches have been proposed, including the numerical simulation of the transport based on a 2D disordered site

model [8], as well as the analytical consideration of the possibility of enhanced backscattering due to the edge spectrum nonlinearity induced by a magnetic field [9] and of interference effects at a disordered edge allowing for loops of the helical edge states [10]. The approach of Ref. [8] gives an adequate description of the conductance suppression phenomenon under the assumption of strong disorder, when the amplitude of a random potential perturbation exceeds the bulk gap energy. The behavior of the conductance under an in-plane field has not been studied in detail, although the numerical simulations [8] also show a suppression of the conductance under the action of such field.

A convenient analytical method for theoretical studies of the edge-state transport in 2D topological insulators is based on the effective Hamiltonian theory, which assumes the reduction of the 2D quantum-mechanical problem, which essentially requires a numerical solution in the presence of a disorder potential, to a 1D problem of electron motion along the edge. The effective  $2 \times 2$  Hamiltonian for edge states [11, 12] has the form  $vk\hat{\sigma}_z$ , where  $v$  is the edge-state velocity,  $k$  is the operator of electron momentum along the edge, and  $\hat{\sigma}_z$  is the Pauli matrix. This Hamiltonian describes two branches of edge states with gapless energy spectrum. However, it does not involve the effects of magnetic field and potential perturbations. Meanwhile, it is well understood [2, 12] that the external magnetic field (or the presence of magnetic impurities in the system) violates the time reversal symmetry and makes the edge states no longer gapless. The gap in the edge state spectrum means that the states with opposite spin projections mix with one another, and, therefore, the electron scattering between counter-propagating states becomes possible. Such a backscattering should reduce the conductance in a similar way as it takes place in constrictions [13] or finite-width strips of 2D topological insulators, where the gap is formed because of the mixing of states from the opposite edges due to the overlap of their wave functions [14]. Therefore, the inclusion of the gap opening effect of a magnetic field into the Hamiltonian of edge states is a necessary step in developing the analytical theory of magnetotransport in 2D topological insulators. The most general form of such  $2 \times 2$  matrix Hamiltonian was proposed in Ref. [12]. It differs from the zero-field case by the presence of an additional term  $\sum_{ij} a_{ij} B_i \hat{\sigma}_j$ , which is linear in components of the magnetic field  $B_i$

(here,  $i$  and  $j$  are Cartesian coordinate indices). For the application of this Hamiltonian to HgTe quantum wells, the coefficients  $a_{ij}$ , which determine the effect of a magnetic field, have been calculated numerically [12]. It is desirable, however, to have a more convenient representation of the effective Hamiltonian, where these coefficients are expressed through the known parameters of the HgTe quantum well system.

The basic goal of the research given in this paper is to develop the all-analytical effective Hamiltonian theory for the 1D motion of electrons in the edge states in the presence of a magnetic field, the spin-orbit interaction, and potential perturbations. The key point of the forthcoming consideration is the transition from the two-subband 2D Hamiltonian of electrons in HgTe quantum wells [2, 5] to an effective 1D Hamiltonian for a couple of edge states. The influence of a magnetic field is taken into account by using perturbation theory. Equation (7) derived in this way is similar to the massive Dirac equation describing the 1D motion of spinless particles with a two-band energy spectrum. The gap between the bands in this spectrum considerably depends on the direction of the magnetic field and vanishes for a special orientation of the field. To show how the presence of the gap influences the ballistic propagation of electrons in the edge states and how the backscattering probability depends on this field, a straightforward application of the theory to standard quantum-mechanical problems, such as the transmission through potential barriers and the motion in a uniform electric field, is carried out. The edge-state transport in random potentials is also discussed. It is demonstrated that the gap in the edge state spectrum leads to a quadratic dependence of the resistance on the magnetic field strength. Some experimental magnetotransport data for 2D topological insulators (in particular, initial quadratic increase of the resistance as a function of the in-plane magnetic field and the dependence of the resistance on the orientation of this field) are explained within the proposed theory.

The paper is organized as follows. Section 2 is devoted to the derivation of an equation for the 1D motion in edge states. The application of this equation to the calculation of transmission and reflection probabilities, which are necessary for the evaluation of the ballistic conductance via edge states, is done in Sec. 3. A discussion relating the results to experimental data on the conductance of 2D topological

insulators based on HgTe quantum wells is presented in Sec. 4.

## 2. Hamiltonian for Edge States

The effective  $4 \times 4$  matrix Hamiltonian describing a 2D insulator phase in a symmetric HgTe quantum well in the basis of two subbands (one of them is the interface-like subband formed as a result of the hybridization of conduction-band states with light hole states and the other is the ground heavy hole subband, with quantization energies  $\varepsilon_1$  and  $\varepsilon_2$ , respectively) was presented in [5] and improved in subsequent works [2, 8, 15, 16] to account for the spin-orbit coupling and magnetic fields. This Hamiltonian is written below in the approximation neglecting inessential small diagonal terms quadratic in the electron momentum:

$$\hat{H} = \begin{pmatrix} U_{\mathbf{r}}^+ + K_z B_z & A\hat{k}_+ & KB_- & -D \\ A\hat{k}_- & U_{\mathbf{r}}^- & D & 0 \\ KB_+ & D & U_{\mathbf{r}}^+ - K_z B_z & -A\hat{k}_- \\ -D & 0 & -A\hat{k}_+ & U_{\mathbf{r}}^- \end{pmatrix}, \quad (1)$$

where  $U_{\mathbf{r}}^{\pm} = \varphi_{\mathbf{r}} \pm \Delta_{\mathbf{r}}/2$ ,  $\mathbf{r} = (x, y)$  is the coordinate in the quantum well plane,  $\varphi_{\mathbf{r}}$  is the electrostatic potential,  $\Delta_{\mathbf{r}} = \varepsilon_1 - \varepsilon_2$  is the gap energy, whose possible variation in the plane is described as  $\Delta_{\mathbf{r}} = \Delta + \delta_{\mathbf{r}}$ , where  $\Delta$  is the averaged gap,  $\hat{k}_{\pm} = \hat{k}_x \pm i\hat{k}_y = -i\partial_x - eB_z y/\hbar c \pm \partial_y$ ,  $e$  is the absolute value of electron charge, and  $B_{\pm} = B_x \pm iB_y$ . To describe the orbital effect of the perpendicular magnetic field  $B_z$ , the vector potential is chosen as  $(-B_z y, 0)$ . The coefficients  $A$ ,  $K$ ,  $K_z$ , and  $D$  are parameters of the effective 2D Hamiltonian. They can be obtained directly by applying the Kane Hamiltonian for the calculation of eigenstates in the quantum well system (see Ref. [16] and references therein). In particular,  $A$  describes the coupling between the subbands at a finite 2D momentum,  $K$  and  $K_z$  characterize the effective Zeeman splitting of the interface-like subband due to in-plane and perpendicular magnetic fields (similar terms for the heavy hole subband are small enough to be neglected), and  $D$  describes the spin-orbit coupling due to the bulk inversion asymmetry. As the upper left and lower right  $2 \times 2$  blocks of the Hamiltonian (1) correspond to the states with opposite projections of the spin, the terms  $D$  and  $KB_{\pm}$  are responsible for the spin mixing.

542

Hamiltonian (1) can be presented in the form  $\hat{H} = \hat{H}_0 + \hat{H}_1$ , where

$$\hat{H}_0 = \begin{pmatrix} \Delta/2 & A\partial_y & 0 & -D \\ -A\partial_y & -\Delta/2 & D & 0 \\ 0 & D & \Delta/2 & A\partial_y \\ -D & 0 & -A\partial_y & -\Delta/2 \end{pmatrix}. \quad (2)$$

Since the 2D system is supposed to be a topological insulator, the case of inverted subband ordering,  $\Delta < 0$ , is considered below. The Hamiltonian  $\hat{H}_0$  describes the states with zero component of the momentum along the  $x$  axis in the absence of potential perturbations  $\varphi_{\mathbf{r}}$ ,  $\delta_{\mathbf{r}}$  and magnetic fields. Assume that there is a boundary at  $y = 0$ , and the 2D system is at  $y > 0$ . The eigenstate problem  $(\hat{H}_0 - \varepsilon)\psi(y) = 0$  has a couple of edge-state solutions with wave functions evanescent from the boundary and energies inside the gap:

$$\begin{pmatrix} 1 \\ -u \\ -i \\ iu \end{pmatrix} e^{-\kappa+(\varepsilon)y}, \quad \begin{pmatrix} 1 \\ -u \\ i \\ -iu \end{pmatrix} e^{-\kappa-(\varepsilon)y}, \quad (3)$$

where  $u = \sqrt{(|\Delta|/2 + \varepsilon)/(|\Delta|/2 - \varepsilon)}$  and  $A\kappa_{\pm}(\varepsilon) = \sqrt{(\Delta/2)^2 - \varepsilon^2 \pm iD}$ . To complete the eigenstate problem, the Hamiltonian  $\hat{H}_0$  should be supplemented with boundary conditions, which allow one to find proper orthogonal combinations of the wave functions (3) and the corresponding eigenvalues of the energy. Without specifying these conditions, let us apply a simplifying assumption that the particle-hole symmetry of the Hamiltonian  $\hat{H}_0$  is retained in the presence of a boundary. This case is realized, for example, if the normal insulator state at  $y < 0$  is described by a Hamiltonian of the same form as Eq. (2), but with large positive  $\Delta$ ; then the boundary conditions take the form [9]  $\psi_1(0) = -\psi_2(0)$  and  $\psi_3(0) = -\psi_4(0)$ , where  $\psi_i$  are the components of the columnar wave function  $\psi$ . Under this assumption, the eigenstates are double degenerate, with the energy  $\varepsilon = 0$ , so  $u = 1$ . Functions (3) are orthogonal to each other under these conditions. It is convenient to form the basis of eigenstates by using the normalized orthogonal combinations of these functions,  $\Psi_1(y)$  and  $\Psi_2(y)$ , according to

$$\Psi_n(y) = C_n \begin{pmatrix} 1 \\ -1 \\ -i \\ i \end{pmatrix} e^{-\kappa+y} + C_n^* \begin{pmatrix} 1 \\ -1 \\ i \\ -i \end{pmatrix} e^{-\kappa-y}, \quad (4)$$

where  $n = 1, 2$  numbers the edge states,

$$C_1 = \frac{\sqrt{\kappa}}{2} \begin{pmatrix} \kappa_+ \\ \kappa_- \end{pmatrix}^{1/4}, \quad C_2 = iC_1, \quad (5)$$

and

$$\kappa_{\pm} = \kappa(1 \pm i\mu), \quad \kappa = \frac{|\Delta|}{2A}, \quad \mu = \frac{2D}{|\Delta|}. \quad (6)$$

The quantity  $\kappa$  is the inverse length of decay of the edge-state wave function from the boundary. The dimensionless parameter  $\mu$  characterizes the spin-orbit coupling strength.

Applying this basis, i.e. searching for a solution of the eigenstate problem with Hamiltonian (1) in the form  $\phi_1(x)\Psi_1(y) + \phi_2(x)\Psi_2(y)$ , one obtains a  $2 \times 2$  matrix equation describing the 1D motion in the edge states:

$$\begin{aligned} (\hat{h} - \varepsilon)\phi(x) &= 0, \\ \hat{h} &= \begin{pmatrix} \varphi_x + i\hbar v \partial_x + vp_0 & g_{\mathbf{B}} \\ g_{\mathbf{B}}^* & \varphi_x - i\hbar v \partial_x - vp_0 \end{pmatrix}, \end{aligned} \quad (7)$$

where  $\phi = (\phi_1, \phi_2)^T$  is the columnar wave function of the edge states, and  $\varphi_x = 2\kappa \int_0^{\infty} dy \varphi_{\mathbf{r}} e^{-2\kappa y}$  is the electrostatic potential acting at the edge. The parameters entering the diagonal part of  $\hat{h}$  are the edge state velocity  $v$  and the momentum displacement  $p_0$  defined as

$$\hbar v = \frac{A}{\sqrt{1 + \mu^2}}, \quad p_0 = \frac{eB_z}{2\kappa c(1 + \mu^2)} + \frac{K_z B_z}{2v\sqrt{1 + \mu^2}}. \quad (8)$$

The complex energy entering the non-diagonal part is linear in the magnetic field:

$$g_{\mathbf{B}} = \frac{KB_x}{2\sqrt{1 + \mu^2}} - i\frac{KB_y}{2} + \frac{\mu ev B_z}{2\kappa c(1 + \mu^2)}. \quad (9)$$

If the magnetic field is directed in the  $(xz)$  plane,  $g_{\mathbf{B}}$  is real. The contribution of the magnetic field to the effective Hamiltonian  $\hat{h}$  has the general form given in Ref. [12]. However, in contrast to Ref. [12], all the parameters are now explicitly related to the quantities entering the Hamiltonian of 2D electrons in HgTe quantum wells, Eq. (1).

The use of the truncated basis  $\Psi_1(y)$  and  $\Psi_2(y)$  (which is actually the key approximation in the derivation of any effective Hamiltonian) provides limitations on applications of Eq. (7). This equation cannot be used in the region of energies beyond the 2D

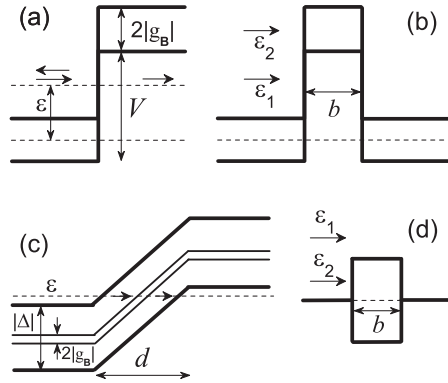
gap,  $|\varepsilon - \varphi_x| > |\Delta|/2$ , where the extended 2D states exist together with the edge states and can mix with them. Such mixing occurs even at  $|\varepsilon - \varphi_x| < |\Delta|/2$ , if the fluctuations of the gap,  $\delta_{\mathbf{r}}$ , are strong. For this reason,  $|\delta_{\mathbf{r}}|$  has to be small compared to  $|\Delta|$ . In fact, the gap fluctuations do not enter Eq. (7), because the latter is obtained in the first order of perturbation theory in the Hamiltonian  $\hat{H}_1$ . The calculation of the second-order contributions leads to additional terms associated with  $\delta_{\mathbf{r}}$ . Such terms can be identified as coordinate-dependent corrections to the quantities  $\kappa$  and  $\mu$  entering  $v$ ,  $p_0$ , and  $g_{\mathbf{B}}$  in Eq. (7). Since these corrections are assumed to be small, Eq. (7) is justified. In spite of the limitations described, expression (8) for the edge state velocity  $v$  is exact (valid for any energy) at  $\mathbf{B} = 0$ .

Equation (7) is similar to the one-dimensional Dirac equation for massive spinless particles. Consider the main properties of this equation. First of all, the terms  $\pm vp_0$  entering the diagonal part of  $\hat{h}$  describe a shift of the electron spectrum in the momentum space, due to the perpendicular magnetic field. These terms have no effect on edge state propagation [9] and can be removed from Eq. (7) by the substitution  $\phi(x) \rightarrow \phi(x) \exp(ip_0 x/\hbar)$  equivalent to a gauge transformation. For this reason, the terms  $\pm vp_0$  in  $\hat{h}$  are omitted below.

The free motion in edge states, when  $\varphi_x = 0$ , is characterized by a constant momentum  $p$  and is described by the energy spectrum

$$\varepsilon_p = \pm \sqrt{v^2 p^2 + |g_{\mathbf{B}}|^2}, \quad (10)$$

which has a gap equal to  $2|g_{\mathbf{B}}|$ . Both the in-plane field and the perpendicular field contribute to the gap. However, the contribution of the perpendicular field appears only due to the orbital effect of this field and in the presence of the spin-orbit coupling [2], when  $\mu \neq 0$ , while the contribution of the in-plane field does not require this coupling [16]. In the case of tilted field with  $B_y = 0$  and  $B_z/B_x = -\kappa c K \sqrt{1 + \mu^2}/ev\mu$ , the gap disappears. Making estimates for a HgTe quantum well 7.3 nm in width ( $|\Delta| \simeq 20$  meV) and assuming  $D \simeq 1$  meV, one finds that the ratio  $B_z/B_x$  corresponding to the zero gap is of the order of unity. The origin of the gap disappearance can be explained as a mutual compensation of the orbital and Zeeman effects of the magnetic field, which are caused by  $B_z$  and  $B_x$ , respectively.



**Fig. 1.** Transmission through a potential step (a), a potential barrier (b), interband transmission in a homogeneous electric field created in a Zener diode structure (c), and the transmission through a magnetic barrier defined by a local gap at  $|x| < b/2$  (d). Solid lines plotted at  $\varphi_x \pm |g_{\mathbf{B}}|$  denote the potential energies of the conduction and valence bands of edge-state 1D electrons; in part (c), the band edges of 2D electrons, at  $\varphi_x \pm |\Delta|/2$ , are also plotted

If the gap is equal to zero, Eq. (7) has two exact solutions:

$$\begin{aligned} \phi^{(1)}(x) &= \begin{pmatrix} e^{-i\Phi_x} \\ 0 \end{pmatrix}, \quad \phi^{(2)}(x) = \begin{pmatrix} 0 \\ e^{i\Phi_x} \end{pmatrix}, \\ \Phi_x &= \frac{1}{\hbar v} \int^x dx' (\varepsilon - \varphi_{x'}). \end{aligned} \quad (11)$$

Since the probability current for the states of Eq. (7) is equal to  $v(|\phi_2(x)|^2 - |\phi_1(x)|^2)$ , these solutions describe the constant probability currents equal to  $-v$  (left-moving) and  $v$  (right-moving), respectively. Regardless to the form of the potential  $\varphi_x$ , there is no backscattering. Thus, the approach presented above relates the topological protection of edge states to a basic property of the massless 1D Dirac model. This property is responsible for the ideal transmission of electrons through potential barriers (Klein paradox [17]), which was observed in graphene at the normal incidence [18, 19]. In the case of nonzero gap, the transmission depends on details of the potential, as illustrated below in some examples of quantum-mechanical problems.

### 3. Propagation of Gapped Edge States

Consider the propagation of electrons in the edge states described by Eq. (7) through finite-size regions with an inhomogeneous electrostatic potential. Sin-

ce the methods of solutions of similar quantum-mechanical problems for the Dirac model are well known [17], and the subject is under the increasing attention in connection with the studies of graphene [18], the details of calculations leading to the results presented below are omitted. The electric current carried by a single edge through an inhomogeneous region is given by  $j = (e/h) \int d\varepsilon T_\varepsilon [f_L(\varepsilon) - f_R(\varepsilon)]$ , where  $f_L$  ( $f_R$ ) are the energy distribution functions of electrons in the edge states on the left (right) sides of the potential perturbation and  $T_\varepsilon$  is the transmission probability related to the reflection probability  $R_\varepsilon$  in the usual way,  $T_\varepsilon + R_\varepsilon = 1$ . The simplest important cases are the following.

*Potential step.* In the case of the potential step ( $\varphi_x = 0$  at  $x < 0$  and  $\varphi_x = V$  at  $x > 0$ ) shown in Fig. 1, a, the transmission of an electron with energy  $\varepsilon$  is nonzero, if  $|V - \varepsilon| > |g_{\mathbf{B}}|$ . Introducing  $\lambda_1 = |g_{\mathbf{B}}|/\varepsilon$  and  $\lambda_2 = |g_{\mathbf{B}}|/(V - \varepsilon)$ , we obtain

$$R_\varepsilon = \frac{|\eta_1 + \eta_2|^2}{|1 + \eta_1 \eta_2|^2}, \quad \eta_i = \frac{\lambda_i}{\sqrt{1 - \lambda_i^2} + 1}. \quad (12)$$

This expression is formally valid also at  $|V - \varepsilon| < |g_{\mathbf{B}}|$ , when  $\eta_2$  is a complex quantity; in this case, the reflection is perfect,  $R_\varepsilon = 1$ . Expression (12) is considerably simplified under the special condition  $\varepsilon = V/2$  (symmetric  $n - p$  junction, as shown in Fig. 1, a):  $R_\varepsilon = 4|g_{\mathbf{B}}|^2/V^2$ . If the gap is small so that  $|\lambda_i| \ll 1$ , the reflection probability is small and quadratic in  $\mathbf{B}$ :  $R_\varepsilon \simeq |g_{\mathbf{B}}|^2 V^2 / [2\varepsilon(V - \varepsilon)]^2$ .

*Potential barrier.* The case  $\varphi_x = 0$  at  $|x| > b/2$  and  $\varphi_x = V$  at  $|x| < b/2$  represents the potential barrier shown in Fig. 1, b. The reflection coefficient is

$$R_\varepsilon = \frac{\sin^2(kb)}{\sin^2(kb) + Q}, \quad Q = \frac{(1 - \lambda_1^2)(1 - \lambda_2^2)}{(\lambda_1 + \lambda_2)^2}, \quad (13)$$

where  $k = \sqrt{(V - \varepsilon)^2 - |g_{\mathbf{B}}|^2}/\hbar v$  is the wavenumber of an electron inside the barrier. If  $|V - \varepsilon| > |g_{\mathbf{B}}|$  ( $\varepsilon = \varepsilon_1$  in Fig. 1, b), electrons can propagate in the barrier region,  $k$  is real, and  $R_\varepsilon$  demonstrates interference oscillations and goes to zero each time when  $kb/\pi$  is integer. Since  $k$  is controlled by the magnetic field, the oscillations can be induced by sweeping  $\mathbf{B}$ . If  $|V - \varepsilon| < |g_{\mathbf{B}}|$  ( $\varepsilon = \varepsilon_2$  in Fig. 1, b), electrons cannot propagate in the barrier region. In this case,  $k$  is imaginary,  $k = i|k|$ ,  $\sin^2(kb) = -\sinh^2(|k|b)$ , and the transmission through sufficiently wide barriers is ex-

ponentially small,  $T_\varepsilon \propto \exp(-2|k|b)$ . If  $|\lambda_i| \ll 1$ , the reflection is small,  $R_\varepsilon \simeq |g_{\mathbf{B}}|^2 V^2 \sin^2(kb) / [\varepsilon(V - \varepsilon)]^2$ .

*Homogeneous electric field.* The motion of a Dirac electron in the potential  $\varphi_x = Fx$  assumes the transition of this electron between the conduction and valence bands in the region near the point  $\varepsilon = \varphi_x$ . For the massless Dirac Hamiltonian, this transition takes place with probability 1. For the massive Dirac Hamiltonian, the electron undergoes the interband (Zener) tunneling, which is formally described within an exactly solvable problem of tunneling through a parabolic barrier [20]. The energy-independent transmission probability is given by the expression

$$T = \exp(-\pi |g_{\mathbf{B}}|^2 / \hbar F v). \quad (14)$$

A similar expression describes the Zener tunneling in graphene at a nonzero angle of incidence [21]. If the magnetic field is weak so that  $|g_{\mathbf{B}}|^2 \ll \hbar F v / \pi$ , one gets a small reflection probability quadratic in the magnetic field,  $R = \pi |g_{\mathbf{B}}|^2 / \hbar F v$ . The homogeneous electric field can be created, for example, in planar  $n - p$  junctions [22] formed in HgTe quantum well structures with split gates, Fig. 1, *c*. In the case of normal insulator, the conductance of such a junction is proportional to  $L_y \exp(-\pi \Delta^2 / 4FA)$ , where  $L_y$  is the sample width. In the case of topological insulator, the edge state transport causes an additional contribution to the conductance [22], which is equal to  $2e^2/h$  in the absence of magnetic fields and can dominate over the normal (bulk) contribution, as the latter is exponentially small at  $\Delta^2 \gg FA$ . If the magnetic field is present, the edge-state contribution is multiplied by a factor of  $T$  from Eq. (14). Since  $F \simeq |\Delta|/d$ , where  $d$  is the length of the inhomogeneous region, the factor in the exponent of Eq. (14) is estimated as  $-2\pi \kappa d |g_{\mathbf{B}}| / \Delta^2$ . For  $d$  on the micrometer scale, one has  $\kappa d \gg 1$ , because  $\kappa^{-1} \sim 30$  nm. This means that, despite the assumed smallness of the ratio  $|g_{\mathbf{B}}|/|\Delta|$ , an exponentially small edge-state transmission in planar  $n - p$  junctions is feasible in the presence of a magnetic field. Therefore, the application of a magnetic field can be used for an efficient control over the current through a Zener diode in the topological insulator state.

Note that Eqs. (12)–(14) coincide with the corresponding results for the one-dimensional Dirac model [17], where  $|g_{\mathbf{B}}|$  plays the role of a “mass parameter”. The reason for this is the following: although

the effective Hamiltonian  $\hat{h}$  is formally different from the one-dimensional Dirac Hamiltonian, it can be reduced to the latter by a unitary transformation.

*Magnetic barrier.* The case of inhomogeneous magnetic field is described by Eq. (7) with  $x$ -dependent  $g_{\mathbf{B}}$ . Consider a rectangular magnetic barrier, implying that the field is absent at  $|x| > b/2$  and finite at  $|x| < b/2$ . This leads to the potential configuration where the gap exists locally at  $|x| < b/2$ , as shown in Fig. 1, *d*. The reflection probability is

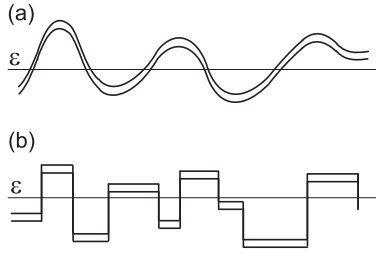
$$R_\varepsilon = \left( 1 + \frac{\hbar^2 v^2 k^2}{|g_{\mathbf{B}}|^2 \sin^2(kb)} \right)^{-1}, \quad (15)$$

where  $k = \sqrt{\varepsilon^2 - |g_{\mathbf{B}}|^2} / \hbar v$ . Similarly to the case of potential barrier, electrons either can or cannot propagate in the barrier region:  $|\varepsilon| > |g_{\mathbf{B}}|$ , real  $k$  or  $|\varepsilon| < |g_{\mathbf{B}}|$ , imaginary  $k$ , respectively. In the first situation, the transmission probability shows interference oscillations, while, in the second one, the transmission can be exponentially small. The model of magnetic barriers is suitable for the description of the electron scattering by magnetic impurities in the absence of a magnetic field. Since the spin-dependent interaction of an electron with such an impurity occurs at a short range, it is natural to assume small  $b$  in Eq. (15) for such applications. If the product  $kb$  is also small, Eq. (15) describes a small energy-independent reflection probability  $R \simeq |g_{\mathbf{B}}|^2 b^2 / \hbar^2 v^2$ .

The validity of the results of this section is determined by the range of applicability of the effective Hamiltonian (7). In particular, the estimate of the second-order perturbation contributions to  $\hat{h}$  allows one to conclude that the results are applicable in the range of magnetic fields, where the energies  $|KB|$  and  $|K_z B_z|$  are small in comparison to  $|\Delta|$ . For HgTe wells, both  $K$  and  $K_z$  are estimated as 1 meV/T, so the results are justified within the 1-T range provided that  $|\Delta| > 10$  meV.

#### 4. Discussion

The opening of the gap in the edge-state spectrum of 2D topological insulators under the action of a magnetic field is the fundamental consequence of the violation of the time reversal symmetry. A one-dimensional quantum-mechanical equation derived in this paper describes the motion of electrons in the edge states under these conditions. The contribution of the in-plane field to the gap energy  $2|g_{\mathbf{B}}|$  arises



**Fig. 2.** Energies of the band extrema for edge-state 1D electrons, given by the expression  $\varphi_x \pm |g_{\mathbf{B}}|$ , in the cases of smooth (a) and sharp (b) random potentials. Electrons with energy  $\epsilon$  experience the multiple Zener tunneling (a) or the multiple transmission across potential steps (b). In both cases, the reflection probability is quadratic in the magnetic field

because of the Zeeman interaction, while the contribution of a perpendicular field exists purely due to the orbital effect of the magnetic field in the presence of the spin-orbit coupling. The gap is sensitive not only to the magnetic field strength, but also to the direction of this field, and vanishes at a special field orientation.

When the gap is present, the scattering of electrons between counter-propagating edge channels can be responsible for the suppression of the ballistic conductance in HgTe quantum well samples. Let us consider a model of transport in a disordered HgTe quantum well near the charge neutrality point, when the Fermi energy is in the middle of the gap between 2D subbands. Since the magnetic field creates a small gap  $2|g_{\mathbf{B}}|$ , an edge-state electron moving in a spatially smooth random potential  $\varphi_x$  (see Fig. 2, a) experiences multiple Zener tunneling events, for which the averaged potential energy tilt  $F$  is estimated as  $2w/l_c$ , where  $w$  is the mean amplitude of the potential variations ( $w$  is assumed to be much larger than  $|g_{\mathbf{B}}|$ ) and  $l_c$  is the mean distance between adjacent local minima and maxima of the random potential. Each tunneling event occurs with a small reflection probability, but the total number of such transitions is large and estimated as  $N = L/l_c$ , where  $L$  is the sample length. Neglecting the interference effects, one may roughly estimate the total reflection probability as  $NR$ , with  $R = 1 - T$  taken from Eq. (14). Then the relative increase in the resistance is expected to be of the order of  $\pi|g_{\mathbf{B}}|^2 L / 2\hbar v w$ . If the magnetic field is perpendicular to the quantum well plane, this dimensionless quantity is estimated as  $2\pi A^3 D^2 L / |\Delta|^4 \ell^4 w$ , where  $\ell = \sqrt{\hbar c / e |B_z|}$  is the magnetic length. Using

$A = 360$  meV nm,  $|\Delta| = 20$  meV,  $D = 1$  meV, and assuming  $w = 3$  meV and  $L = 2$   $\mu$ m, the relative increase in the resistance is given by  $2.5[B_z(\text{T})]^2$ . If the random potential is sharp, as shown in Fig. 2, b, the electron is transmitted across a number of potential steps, and the relative increase in the resistance is estimated as  $|g_{\mathbf{B}}|^2 L / w^2 l_c$ , where  $l_c$  is now the average distance between potential steps. Assuming  $l_c \simeq 10$  nm, one gets a stronger effect of the magnetic field on the resistance compared to the case of smooth random potential. However, the model of smooth potential seems to be a more realistic one.

Therefore, according to the theory described in this paper, the increase in the resistance is proportional to the square of the magnetic field and becomes essential in the fields of the order of 1 T. Since the contributions of the in-plane field and the perpendicular field to the gap energy are comparable (see Sec. 2), the effect of both fields on the backscattering should be similar. In agreement with this theory, the numerical simulations of the transport within a 2D disordered site model [8] show a weak, quadratic in the magnetic field, increase in the resistance in the case of weak disorder. For a strong disorder, when the potential amplitude exceeds the bulk gap energy, the simulation gives a completely different result: a strong, linear in  $B_z$ , increase in the resistance and a much weaker effect of the in-plane field. Since it is the behavior actually observed experimentally, one may conclude that the strong disorder is a necessary precondition for the dramatic influence of a perpendicular magnetic field on the ballistic resistance and that the strong disorder is present in the samples investigated. The case of strong disorder, when the transitions of electrons between the edge and bulk states are possible, is beyond the range of validity of the effective Hamiltonian theory.

On the other hand, the theory can explain the observed [3, 6] increase in the resistance under the in-plane magnetic field of the order of 1 T. This increase apparently begins with a quadratic field dependence and is sensitive to the gate voltage controlling the position of the Fermi energy in the bulk gap [6]. Moreover, the dependence of the resistance on the orientation of the in-plane field shows (Ref. [3], p. 68) that the field perpendicular to the current leads to a stronger effect. This is in agreement with the theory demonstrating that the field  $B_y$  creates a larger gap than the field  $B_x$ , see Eq. (9). The difference is

controlled by the parameter  $\mu = 2D/|\Delta|$ , which is not small in the case where the bulk gap  $|\Delta|$  is of the order of 1 meV. Indeed, a considerable dependence of the resistance on the orientation of the field has been observed [3] for a sample with a small bulk gap. Numerical simulations [8], carried out for  $\mu \ll 1$ , show a negligible orientation dependence, in agreement with the theory.

In summary, the parameters of the effective Hamiltonian for edge states in two-dimensional topological insulators based on HgTe quantum wells are calculated analytically. The effect of magnetic fields on the quantum-mechanical properties of these states in the presence of potential perturbations is studied. The feasibility of a broad control over the ballistic transport of edge-state electrons by magnetic fields is demonstrated. The results of the effective Hamiltonian theory are compared to both experimental findings and numerical simulation data on the magnetoresistance of HgTe quantum wells. The theory explains the observed behavior of the resistance under an in-plane magnetic field, but does not explain the strong linear increase in the resistance as a response to a perpendicular magnetic field. This increase is likely caused by the transitions of electrons between edge and bulk states, which are not accounted by the effective Hamiltonian theory and are possible in the presence of a high-amplitude disorder potential.

*I thank the anonymous Referee for the attentive consideration of the article and for the useful remarks, which helped me to improve the text.*

1. M. König, S. Wiedmann, C. Brüne, A. Roth, H. Buhmann, L.W. Molenkamp, X.L. Qi, and S.C. Zhang, *Science* **318**, 766 (2007).
2. M. König, H. Buhmann, L.W. Molenkamp, T.L. Hughes, C.-X. Liu, X.-L. Qi, and S.-C. Zhang, *J. Phys. Soc. Japan* **77**, 031007 (2008).
3. M. König, *Ph.D. thesis*, (Würzburg, 2007).
4. A. Roth, C. Brüne, H. Buhmann, L.W. Molenkamp, J. Maciejko, X.-L. Qi, and S.-C. Zhang, *Science* **325**, 294 (2009).
5. B.A. Bernevig, T.L. Hughes, and S.C. Zhang, *Science* **314**, 1757 (2006).
6. G.M. Gusev, Z.D. Kvon, O.A. Shegai, N.N. Mikhailov, S.A. Dvoretzky, and J.C. Portal, *Phys. Rev. B* **84**, 121302(R) (2011).
7. G.M. Gusev, E.B. Olshanetsky, Z.D. Kvon, N.N. Mikhailov, and S.A. Dvoretzky, *Phys. Rev. B* **87**, 081311(R) (2013).

8. J. Maciejko, X.L. Qi, and S.C. Zhang, *Phys. Rev. B* **82**, 155310 (2010).
9. G. Tkachov and E.M. Hankiewicz, *Phys. Rev. Lett.* **104**, 166803 (2010).
10. P. Delplace, J. Li, and M. Büttiker, *Phys. Rev. Lett.* **109**, 246803 (2012).
11. X.-L. Qi and S.-C. Zhang, *Rev. Mod. Phys.* **83**, 1057 (2011).
12. X.L. Qi, T.L. Hughes, and S.C. Zhang, *Nature Phys.* **4**, 273 (2008).
13. V. Krueckl and K. Richter, *Phys. Rev. Lett.* **107**, 086803 (2011).
14. B. Zhou, H.-Z. Lu, R.-L. Chu, S.-Q. Shen, and Q. Niu, *Phys. Rev. Lett.* **101**, 246807 (2008).
15. D.G. Rothe, R.W. Reintaler, C.X. Liu, L.W. Molenkamp, S.C. Zhang, and E.M. Hankiewicz, *New J. Phys.* **12**, 065012 (2010).
16. O.E. Raichev, *Phys. Rev. B* **85**, 045310 (2012).
17. A. Calogeracos and N. Dombey, *Contemp. Phys.* **40**, 313 (1999).
18. S. Das Sarma, S. Adam, E.H. Hwang, and E. Rossi, *Rev. Mod. Phys.* **83**, 407 (2011).
19. R.N. Sajjad, S. Sutar, J.U. Lee, and A.W. Ghosh, *Phys. Rev. B* **86**, 155412 (2012).
20. L.D. Landau and E.M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon Press, New York, 1977).
21. V.V. Cheianov and V.I. Falko, *Phys. Rev. B* **74**, 041403 (2006).
22. L.B. Zhang, K. Chang, X.C. Xie, H. Buhmann, and L.W. Molenkamp, *New J. Phys.* **12**, 083058 (2010).

Received 30.09.14

*О.Е. Райчев*

#### ЕФЕКТИВНИЙ ГАМІЛЬТОНІАН І ДИНАМІКА КРАЙОВИХ СТАНІВ В ДВОВИМІРНИХ ТОПОЛОГІЧНИХ ІЗОЛЯТОРАХ В МАГНІТНИХ ПОЛЯХ

Р е з ю м е

Магнітне поле відкриває щілину в спектрі крайових станів двовимірних топологічних ізоляторів, завдяки чому руйнується захист цих станів від розсіювання назад. Щоб пов'язати властивості цієї щілини з параметрами системи та вивчити динаміку електронів в крайових станах при наявності неоднорідних потенціалів, розроблена теорія ефективного гамільтоніана. Ця аналітична теорія застосована для розгляду квантово-механічних проблем проходження електронів в крайових станах крізь потенціальні сходинки і бар'єри та руху в постійному електричному полі. Вплив магнітного поля на опір двовимірних топологічних ізоляторів на основі HgTe квантових ям обговорено разом з порівнянням до експериментальних даних.



*О.Э. Райчев*

ЭФФЕКТИВНЫЙ ГАМИЛЬТониАН  
И ДИНАМИКА КРАЕВЫХ СОСТОЯНИЙ  
В ДВУХМЕРНЫХ ТОПОЛОГИЧЕСКИХ  
ИЗОЛЯТОРАХ В МАГНИТНЫХ ПОЛЯХ

Резюме

Магнитное поле открывает щель в спектре краевых состояний двухмерных топологических изоляторов, вследствие чего разрушается защита этих состояний от рассеяния на-

зад. Чтобы связать свойства этой щели с параметрами системы и изучить динамику электронов в краевых состояниях при наличии неоднородных потенциалов, развита теория эффективного гамильтониана. Эта аналитическая теория применена для рассмотрения квантово-механических проблем прохождения электронов в краевых состояниях сквозь потенциальные ступеньки и барьеры, а также движения в постоянном электрическом поле. Влияние магнитного поля на сопротивление двухмерных топологических изоляторов на основе HgTe квантовых ям обсуждено и проведено сравнение с экспериментальными данными.