Splitting of Dirac cones in HgTe quantum wells: Effects of crystallographic orientation, interface-, bulk-, and structure-inversion asymmetry

M. V. Durnev, G. V. Budkin, and S. A. Tarasenko
Ioffe Institute, 194021 St. Petersburg, Russia

We develop a microscopic theory of the fine structure of Dirac states in (0lh)-grown HgTe/CdHgTe quantum wells (QWs), where \( l \) and \( h \) are the Miller indices. It is shown that bulk, interface, and structure inversion asymmetry causes the anticrossing of levels even at zero in-plane wave vector and lifts the Dirac state degeneracy. In the QWs of critical thickness, the two-fold degenerate Dirac cone gets split into non-degenerate Weyl cones. The splitting and the Weyl point positions dramatically depend on the QW crystallographic orientation. We calculate the splitting parameters related to bulk, interface, and structure inversion asymmetry and derive the effective Hamiltonian of the Dirac states. Further, we obtain an analytical expression for the energy spectrum and discuss the spectrum for (001)-, (013)- and (011)-grown QWs.

I. INTRODUCTION

Heterostructures containing band-inverted compound HgTe are in the focus of modern research in solid state physics. Depending on heterostructure design, particularly the thickness of HgTe layer, they host a variety of phases including the phases of three-dimensional and two-dimensional (2D) topological insulators, 2D gapless semiconductor, 2D semimetal, etc. Of special interest is the 2D gapless phase with linear-dispersion Dirac fermions that is realized in HgTe quantum wells (QWs) of critical thickness, i.e., at the point of trivial insulator – topological insulator transition.\(^{33}\)

In the model of centrosymmetric heterostructure, the Dirac cones in HgTe/CdHgTe QWs are 2-fold degenerate yielding the 4-fold degenerate Dirac point at \( k = 0 \) in the QW of critical thickness.\(^{34}\) Here, \( k \) is the in-plane wave vector. Bulk inversion asymmetry (BIA) related to the lack of an inversion center in host zinc-blend crystal, interface inversion asymmetry (IIA) related to anisotropy of chemical bonds at interfaces, and structure inversion asymmetry (SIA) lift the Dirac state degeneracy.\(^{35}\) This splitting is contributed by canonical \( k \)-linear Rashba\(^{13,19}\) and Dresselhaus\(^{14,20}\) terms as well as the term lifting the 4-fold degeneracy at \( k = 0 \). The anticrossing gap at \( k = 0 \) was found to be quite large in (001)-grown QWs and originates mostly from light-hole–heavy-hole mixing at the QW interfaces.\(^{31,12}\)

Many experiments, however, are being carried out on HgTe/CdHgTe structures grown along low-symmetry crystallographic directions, such as [013] and [012], see Refs. 10–12, 21–23. The choice of crystallographic orientations is dictated by technology: MBE growth of HgTe on GaAs surface enables one to obtain high-quality structures is Val′kin et al.\(^{27,28}\) and CdHgTe layers on low-symmetry (lattice-mismatch) GaAs substrate enables one to obtain high-quality structure.\(^{29}\) This motivates theoretical studies of low-symmetry QWs.\(^{33,25,30}\)

Here, we develop a microscopic theory of the fine structure of Dirac states in HgTe/CdHgTe QWs taking account IIA, BIA, and SIA coupling. We show that the energy spectrum in the QW of the critical thickness dramatically depends on the QW crystallographic orientation and calculate the splitting parameters. We explore the class of (0lh)-grown QWs, where \( l \) and \( h \) are the Miller indices, and study how the fine structure evolves from (001)- to (013)-, and (011)-grown QWs.

II. FINE STRUCTURE OF DIRAC STATES

The Dirac states in HgTe/CdHgTe QWs of critical and close-to-critical thickness are formed from the electron-like \(|E_1, \pm 1/2\rangle\) and heavy-hole \(|H_1, \pm 3/2\rangle\) states.\(^{27,28}\) The corresponding basis functions at \( k = 0 \) have the form

\[
|E_1, +1/2 \rangle = f_1(z) |\Gamma_6, +1/2 \rangle + f_3(z) |\Gamma_8, +1/2 \rangle , \\
|H_1, +3/2 \rangle = f_3(z) |\Gamma_8, +3/2 \rangle , \\
|E_1, -1/2 \rangle = f_1(z) |\Gamma_6, -1/2 \rangle + f_3(z) |\Gamma_8, -1/2 \rangle , \\
|H_1, -3/2 \rangle = f_3(z) |\Gamma_8, -3/2 \rangle ,
\]

where \( k = (k_x, k_y) \) is the in-plane wave vector, \( f_j(z) (j = 1, 3, 4) \) are the envelope functions, \( z \) is the growth direction, \( |\Gamma_6, m \rangle \) \((m = \pm 1/2)\) and \( |\Gamma_8, m \rangle \) \((m = \pm 1/2, \pm 3/2)\) are the Bloch amplitudes of the \( \Gamma_6 \) and \( \Gamma_8 \) bands, respectively, in the Brillouin zone center. We consider (0lh)-oriented QWs and use the QW-related coordinate frame \( x \parallel [100], y \parallel [0l0], \) and \( z \parallel [00h] \).

The effective 4 \times 4 Hamiltonian, which describes the coupling of the basis states and formation of the Dirac-like spectrum, can be derived in the \( k \cdot p \) theory, see Sec. III. Taking into account bulk, structure, and interface inversion asymmetry in (0lh)-grown QWs, one can present the effective Hamiltonian in the form

\[
H = H_0 + H_{\text{IIA/BIA}} + H_{\text{SIA}},
\]

where

\[
H_0 = \begin{pmatrix}
\delta & iA_k^+ & 0 & 0 \\
-iA_k^- & -\delta & 0 & 0 \\
0 & 0 & \delta & iA_k^- \\
0 & 0 & iA_k^+ & -\delta
\end{pmatrix}
\]

is the \( k \)-linear Bernevig-Hughes-Zhang Hamiltonian (2D Dirac Hamiltonian)\(^{27}\) \( A \) is a parameter determining the velocity of Dirac fermions, \( \delta \) is the energy distance between the \( E_1 \) and \( H_1 \) subbands in the absence of mixing.

Interface inversion asymmetry related to anisotropy of chemical bonds at the interfaces and bulk inversion asymmetry related to the lack of inversion center in host crystal
lead to a mixing of the basis states. This mixing at \( k = 0 \) is described by the Hamiltonian

\[
H_{\text{IIA/BIA}} = \begin{pmatrix}
0 & -\eta \sin 2\theta & 0 & i\gamma \cos 2\theta \\
-\eta \sin 2\theta & 0 & i\gamma \cos 2\theta & 0 \\
0 & -i\gamma \cos 2\theta & 0 & \eta \sin 2\theta \\
i\gamma \cos 2\theta & 0 & \eta \sin 2\theta & 0
\end{pmatrix},
\]

where \( \eta \) and \( \gamma \) are mixing parameters, \( \theta = \arctan(l/h) \) is the angle between the QW growth direction [0lh] and the [001] axis. The angles \( \theta = 0 \), \( \arctan(1/3) \approx 0.321 \), and \( \pi/4 \) correspond to [001], [013], and [011] growth directions, respectively.

Structure inversion asymmetry in (0lh)-oriented QWs grown from cubic materials also mixes the basis states at \( k = 0 \), which is described by the Hamiltonian

\[
H_{\text{SIA}} = \begin{pmatrix}
0 & i\chi \sin 4\theta & 0 & \zeta \sin^2 2\theta \\
-i\chi \sin 4\theta & 0 & \zeta \sin^2 2\theta & 0 \\
0 & \zeta \sin^2 2\theta & 0 & i\chi \sin 4\theta \\
\zeta \sin^2 2\theta & 0 & -i\chi \sin 4\theta & 0
\end{pmatrix}.
\]

The mixing parameters \( \chi \) and \( \zeta \) are nonzero if both structure inversion asymmetry and the cubic shape of lattice unit cells are taken into account. Note also that \( H_{\text{SIA}} \) vanishes in (001)-grown QWs.

The parameters \( \eta, \gamma, \chi, \) and \( \zeta \) are calculated in Sec. [III] in the framework of the 6-band \( k \cdot p \) model. An estimation for HgTe/Cd_{0.7}Hg_{0.3}Te QWs with the critical thickness \( d_c \approx 6.7 \) nm gives \( \eta, \gamma \sim 5 \) meV and \( \zeta, \chi \sim 0.1 \) meV in the electric field \( E_z = 15 \) kV/cm.

The Hamiltonians \( H_{\text{IIA/BIA}} \) and \( H_{\text{SIA}} \) depend on the QW growth direction defined by the \( \theta \) angle. Straightforward diagonalization of the Hamiltonian \( H_{\text{IIA/BIA}} \) yields four dispersion branches

\[
E_{1,4} = \mp \sqrt{\delta^2 + \eta_0^2 + \eta_0^2 + \zeta_0^2 + \chi_0^2 + A^2 k^2 \mp 2AK},
\]

\[
E_{2,3} = \mp \sqrt{\delta^2 + \eta_0^2 + \eta_0^2 + \zeta_0^2 + \chi_0^2 + A^2 k^2 \mp 2AK},
\]

where \( k^2 = k_x^2 + k_y^2 \),

\[
K = \sqrt{(\eta_0^2 + \zeta_0^2)k^2 + (\eta_0 k_x + \eta_0 k_y)^2},
\]

and

\[
\gamma_\theta = \gamma \cos 2\theta, \quad \eta_0 = \eta \sin 2\theta, \\
\zeta_\theta = \zeta \sin^2 2\theta, \quad \chi_\theta = \chi \sin 4\theta.
\]

In the following subsections we analyze the fine structure of Dirac states in QWs with different crystallographic orientations for different mixing mechanisms.

### A. Interface and bulk inversion asymmetry

Dirac states in HgTe/CdHgTe QWs with symmetric confinement potential are described by the Hamiltonian \( H = H_0 + H_{\text{IIA/BIA}} \) with \( H_0 \) and \( H_{\text{IIA/BIA}} \) given by Eqs. [3] and [4], respectively. In this case, Eq. [6] yields

\[
E_{1,4} = \mp \sqrt{\delta^2 + \gamma_\theta^2 + \gamma_\theta^2 + A^2 k^2 + 2A \sqrt{\gamma_\theta^2 k^2 + \eta_0^2 k_y^2}},
\]

\[
E_{2,3} = \mp \sqrt{\delta^2 + \gamma_\theta^2 + \gamma_\theta^2 + A^2 k^2 - 2A \sqrt{\gamma_\theta^2 k^2 + \eta_0^2 k_y^2}}.
\]

![FIG. 1](image1.png)

FIG. 1. Energy spectra of Dirac states in (001)-, (013)- and (011)-grown HgTe/CdHgTe QWs of critical thickness with interface- and bulk-inversion asymmetry included. The spectra are calculated after Eq. [9] for \( \delta = 0 \) and \( \gamma = \eta = 2\delta \). Color decodes the pseudospin projection onto the QW normal (see text for details): blue and red correspond to \( \sigma_z = -1 \) and \( \sigma_z = +1 \), respectively, whereas purple corresponds to \( \sigma_z = 0 \).

![FIG. 2](image2.png)

FIG. 2. Energy spectra of Dirac states in (001)-, (013)- and (011)-grown HgTe/CdHgTe QWs of close-to-critical thickness with interface- and bulk-inversion asymmetry included. The spectra are calculated after Eq. [9] for \( \gamma = \eta = 2\delta \). Color decodes the pseudospin projection onto the QW normal: blue and red correspond to \( \sigma_z = -1 \) and \( \sigma_z = +1 \), respectively, whereas purple corresponds to \( \sigma_z = 0 \).

Figure [4] shows the energy spectra of Dirac states in (001), (013), and (011) QWs of critical thickness (\( \delta = 0 \)) with the IIA/BIA term included. The (001) orientation corresponds to \( \theta = 0 \). In this case, the energy spectrum consists of two non-degenerate (Weyl) cones shifted vertically (along the energy axis) with respect to each other. The Weyl points are located at \( k = 0 \) and the energies \( E = \pm \gamma \). The (011) orientation corresponds to \( \theta = \pi/4 \).
In such QWs, the IIA/BIA interaction splits the Dirac cone into two Weyl cones shifted along \( k_y \) with respect to each other. The Weyl points are located at \( k = (0, \pm \eta/A) \). The spectrum in (013) and general (0lh) QWs is an intermediate case between the spectra in (001) and (011) structures. Now, there are four Weyl points in the energy spectrum. Two points are located at \( k = (0, \pm |\sqrt{\frac{\delta}{2}} + \frac{\eta}{A}/A) \) and zero energy, while the other two points are at \( k = 0 \) and the energies \( E = \pm \sqrt{|\delta^2 + \frac{\eta^2}{A}|} \).

The color in Fig. 1 decodes the projection of pseudospin onto the QW normal \( \sigma_z \) defined by \( \sigma_z = |c_1|^2 + |c_2|^2 - |c_3|^2 - |c_4|^2 \), where \( c_j \) are the coefficients of decomposition of a wave function \( \psi \) over the basis functions \( \{ |E_1, +1/2 \rangle \) and \( |H_1, +3/2 \rangle \) and “spin-down” blocks in the given state \( \psi \). In (001) QWs, the Weyl cones are formed by the “spin-up” and “spin-down” blocks in equal portions and \( \sigma_z = 0 \) (purple color) for all eigenstates. In contrast, the split Weyl cones in (011) QWs are formed by pure “spin-up” and “spin-down” states and characterized by \( \sigma_z = +1 \) (red color) and \( \sigma_z = -1 \) (red color) pseudospin projections.

The energy spectra of (001), (013), and (011) QWs of close-to-critical thickness (with the gap \( 2|\delta| \)) are shown in Fig. 2. In (001) QWs, the spectrum is given by \( E = \pm \sqrt{\delta^2 + (A|k| + \gamma)^2} \) and the band extrema are situated at the loop with \( |k| = |\gamma/A| \). In (011) QWs, the spectrum has the form \( E = \pm \sqrt{\delta^2 + A^2 k_x^2 + (A |k_y| + \eta)^2} \) and consists of the branches with the \( \sigma_z = \pm 1 \) pseudospin projections. In general case of (0lh) orientation, e.g., (013), the band extrema are situated at the points \( k = (0, \pm \sqrt{\frac{\delta}{2}} + \frac{\eta}{A}/A) \). The contours of constant energy are toric sections, in particular, at \( |E| > \sqrt{\delta^2 + \frac{\eta^2}{A}/A} \), the isoenergy contours are ovals elongated along \( k_y \).

B. Structure inversion asymmetry

Here, we study the influence of structure inversion asymmetry on the energy spectrum of Dirac states. For this purpose, we consider the Hamiltonian \( \hat{H} = \hat{H}_0 + \hat{H}_{\text{SIA}} \) with \( \hat{H}_0 \) and \( \hat{H}_{\text{SIA}} \) given by Eqs. (3) and (5), respectively. In this case, Eq. (6) yields

\[
E_{1,4} = \pm \sqrt{\delta^2 + \zeta_0^2 + \chi_0^2 + A^2 k^2 + 2 A \sqrt{\delta^2 k_2^2 + \chi_0^2 k_2^2}}, \\
E_{2,3} = \pm \sqrt{\delta^2 + \zeta_0^2 + \chi_0^2 + A^2 k^2 - 2 A \sqrt{\delta^2 k_2^2 + \chi_0^2 k_2^2}}.
\]

(10)

Figure 3 shows the energy dispersions given by Eq. (10) for (001), (013), and (011) QWs of critical thickness (\( \delta = 0 \)). In (001) QWs, structure inversion asymmetry does not contribute to the mixing of the basis states at \( k = 0 \). As a result, the point \( k = 0 \) remains four-fold degenerate just as it is in the Bernevig-Hughes-Zhang model. In QWs of other orientations, the SIA interaction lifts the four-fold degeneracy at \( k = 0 \) and splits the Dirac cone.

Generally, there are four Weyl points in the energy spectrum located at \( k = (\pm \sqrt{\frac{\delta}{2}} + \frac{\eta}{A}/A, 0) \) and zero energy and at \( k = 0 \) and the energies \( E = \pm \sqrt{\delta^2 + \frac{\eta^2}{A}/A} \), respectively. Interestingly, the SIA interaction in (011) QWs splits the Dirac cone in a way similar to the IIA/BIA interaction does in (001) QWs.

In QW structures with a gap (not shown), the band extrema are located at \( k = (\pm \sqrt{\frac{\delta}{2}} + \frac{\eta}{A}/A, 0) \), in particular, at \( k = 0 \) in (001) QWs and at the loop with \( |k| = |\zeta/A| \) in (011) QWs.

C. Interplay of IIA/BIA and SIA

In real QW structures, all types of asymmetry, including bulk, interface, and structure inversion asymmetry, are present. The dispersion branches in that case are given by the general Eq. (6). Figure 4 shows the energy spectra of Dirac states in such QWs with asymmetric confinement potential and grown along different crystallographic orientations.

In (001) QWs, the splitting of the Dirac cone at \( k = 0 \) is determined by the BIA/IIA term and the energy spectrum coincides with the one shown in Fig. 1. The spectrum of asymmetric (011) QWs is qualitatively similar to the spectrum of symmetric (013) QWs. There are four Weyl points: two of them located at \( k = (\pm \sqrt{\frac{\delta}{2}} + \frac{\eta}{A}/A, 0) \) and zero energy and the other two located at \( k = 0 \) and the energies \( E = \pm \sqrt{\frac{\delta^2}{2} + \frac{\eta^2}{A}} \).

The spectrum of a general (0lh)-grown QW with asymmetric confinement potential is shown in the central panel in Fig. 4. The Weyl points at zero energy are located at the wave vectors

\[
k = \pm \sqrt{\frac{\gamma_0^2 + \eta_0^2 + \zeta_0^2 + \chi_0^2}{A^2 (\eta_0^2 + \chi_0^2)}} (\chi_0, \eta_0).
\]

Interestingly, the position of these points in the \( k \) space is not pinned to a specific in-plane direction. The angle between the line connecting the Weyl points and the \( k_x \)
axis, \( \arctan(\eta_\theta/\chi_\theta) \), depends on the SIA parameter \( \chi \) and, therefore, can be controlled by an external electric field applied along the QW normal, e.g., by gate voltage.

\[ \mathcal{H}_{\text{68}} \text{ blocks to the second order in the wave vector } \mathbf{k} \text{ have the form} \]

\[ \mathcal{H}_{68}^{\text{kp}} = U_6 + \frac{\hbar^2 k^2}{2m_e} , \]

\[ \mathcal{H}_{88}^{\text{kp}} = U_8 + \frac{\hbar^2}{2m_0} \left[ -\left( \gamma_1' + \frac{5}{2} \gamma_2' \right) k^2 + 2\gamma_2'(Jk)^2 + +2(\gamma_3' - \gamma_2') \sum_{i \neq j} \{ J_i J_j \}_{ik} k_j \right] + \frac{4\sqrt{3} \mathcal{V}}{\sqrt{3}} \mathbf{V} \mathbf{k} , \]

where \( U_6 \) and \( U_8 \) are the energies of the \( \Gamma_6 \) and \( \Gamma_8 \) bands at \( \mathbf{k} = 0 \), \( \mathbf{k} = (k_x', k_y', k_z') \) is the wave vector, \( \gamma_1' \), \( \gamma_2' \), \( \gamma_3' \), and \( m_0' \) are the contributions to the Luttinger parameters and the effective mass, respectively, from remote bands and free electron dispersion, \( J = (J_x', J_y', J_z') \) is the vector composed of the momentum-3/2 matrices, \( \mathcal{V} = (V_x', V_y', V_z') \), where \( V_x' = (J_x', J_y', J_z' - J_{2z}) \) and the other components of \( \mathcal{V} \) are derived by the cyclic permutation of the subscripts, \( \{ A, B \}_s = (AB + BA)/2 \) is the symmetrized product of the operators \( A \) and \( B \), and \( \gamma_0 \) is a band parameter.

To construct the \( \mathcal{H}_{68} \) block, one notes that the direct product \( \Gamma_6 \times \Gamma_8 \) is decomposed into the irreducible representations \( \Gamma_3 + \Gamma_4 + \Gamma_5 \). The sets \{ \( k_x', k_y', k_z' \) \} and \{ \( k_x', k_y', k_z', k_{x'}, k_{y'} \) \} transform according to the vector representation \( \Gamma_5 \) whereas the pair \{ \( 2k_x'^2 - k_y'^2 - k_z'^2, \sqrt{3}(k_x'^2 - k_y'^2) \) \} transforms according to the \( \Gamma_3 \) representation. The combinations that transform according to the pseudo-vector representation \( \Gamma_4 \) are cubic in \( \mathbf{k} \) and are not considered. Thus, the \( \mathcal{H}_{68}^{\text{kp}} \) block is given by \[ \mathcal{H}_{68}^{\text{kp}} = \left( \begin{array}{ccc}
\frac{1}{\sqrt{3}}(P_{+} k_{+} k_{-} - P k_{-}) & \frac{1}{3\sqrt{2}} B_{-}(2k_{+}^2 - k_{-}^2) \\
\sqrt{\frac{2}{3}}(iP_{k_{+}} + B_{+} k_{+} k_{y'}) & \frac{1}{\sqrt{6}} B_{-}(k_{+}^2 - k_{-}^2) \\
\frac{1}{\sqrt{6}}(P_{k_{+}} + B_{+} k_{-} k_{y'}) & \sqrt{\frac{2}{3}}(iP_{k_{+}} + B_{+} k_{+} k_{y'}) \\
\frac{1}{3\sqrt{2}} B_{-}(k_{+}^2 - 2k_{-}^2) & \frac{1}{\sqrt{2}}(P_{+} k_{+} + B_{+} k_{-} k_{-})
\end{array} \right) \]

where \( P = i(\hbar/m_0)\mathcal{P}_z \) is the Kane matrix element, \( B_{\pm} \) are band parameters, \( k_{\pm} = k_x' \pm ik_y' \), and \( k_{\pm}^2 = k_{x'}^2 + k_{y'}^2 \). Note that the definition of \( P \) and \( B \) in Eq. \( 15 \) differs by the factor of \( i \) from that in Ref. \[30\].

The extended Kane Hamiltonian given by the blocks \( \mathcal{H}_{68}^{\text{kp}} \) reflects the real symmetry of the zinc-blende lattice including its cubic shape and the lack of space inversion center. The isotropic centrosymmetric approximation corresponds to \( \gamma_3' = \gamma_2', \gamma_0 = 0 \), and \( B_{\pm} = 0 \). The nonzero difference \( \gamma_3' - \gamma_2' \) takes into account the cubic anisotropy of the unit cell whereas the nonzero parameters \( \gamma_0 \) and \( B_\pm \) reflect bulk inversion asymmetry. The \( B_- \) parameter couples the functions with the opposite spin projections and, hence, is expected to be smaller than \( B_+ \). We neglect this parameter in the following calculations.
The parameters of the effective 6-band Hamiltonian \( \mathcal{H}_{\text{def}} \) can be expressed via the coupling parameters and the energy gaps in multi-band \( k\cdot p \) theory. The results of such calculations in the 14-band \( k\cdot p \) model \cite{19,19,19,19,19} which includes the \( \Gamma_7 \) valence band and the remote \( \Gamma_6 \) and \( \Gamma_8 \) conduction bands in addition to the considered \( \Gamma_6 \) and \( \Gamma_8 \) bands, are summarized in Tab. I.

Layers in epitaxial HgTe/CdHgTe structures are typically strained because of considerable mismatch (of about 0.3\%) between HgTe and CdTe lattice constants. The layers in epitaxial HgTe/CdHgTe structures are typically strained because of considerable mismatch (of about 0.3\%) between HgTe and CdTe lattice constants. The layers in epitaxial HgTe/CdHgTe structures are typically strained because of considerable mismatch (of about 0.3\%) between HgTe and CdTe lattice constants. The layers in epitaxial HgTe/CdHgTe structures are typically strained because of considerable mismatch (of about 0.3\%) between HgTe and CdTe lattice constants. The layers in epitaxial HgTe/CdHgTe structures are typically strained because of considerable mismatch (of about 0.3\%) between HgTe and CdTe lattice constants.

The parameters of the effective 6-band Hamiltonian \( \mathcal{H}_{\text{def}} \) can be constructed in a way similar to the \( k\cdot p \) Hamiltonian. Such a procedure yields the diagonal blocks

\[
\mathcal{H}_{66}^{\text{def}} = \Xi_c \text{Tr} \epsilon ,
\]

\[
\mathcal{H}_{88}^{\text{def}} = \left( a + \frac{5}{4} b \right) \text{Tr} \epsilon - b \sum_{i,j} \{ J_i J_j \} s \epsilon_{ij} + \left( b - \frac{d}{\sqrt{3}} \right) \sum_{i \neq j} \{ J_i J_j \} s \epsilon_{ij} ,
\]

where \( \Xi_c \) is the \( \Gamma_6 \)-band deformation potential, \( a, b, \) and \( d \) are the \( \Gamma_1 \)-band deformation potentials, \( \mathcal{H}_{88}^{\text{def}} \) is the Bir-Pikus Hamiltonian, \( \epsilon \) is the strain tensor, and the off-diagonal blocks

\[
\mathcal{H}_{68}^{\text{def}} = \begin{pmatrix}
-\Xi_{cv} \frac{\epsilon_{x'y'} - \epsilon_{xz'}}{\sqrt{2}} & i\Xi_{cv} \frac{2\epsilon_{x'z'} - \epsilon_{x'z'} - \epsilon_{y'y'}}{3\sqrt{2}} \\
\sqrt{2} \Xi_{cv} \epsilon_{x'y'} & -\Xi_{cv} \frac{\epsilon_{y'z'} - \epsilon_{x'z'}}{\sqrt{6}} + i\Xi_{cv} \frac{\epsilon_{x'z'} - \epsilon_{y'y'}}{\sqrt{6}} \\
\Xi_{cv} \frac{\epsilon_{x'z'} + \epsilon_{y'y'}}{\sqrt{6}} & -\Xi_{cv} \frac{\epsilon_{y'z'}}{\sqrt{6}} - i\Xi_{cv} \frac{\epsilon_{x'z'} - \epsilon_{y'y'}}{\sqrt{6}} \\
i\Xi_{cv} \frac{\epsilon_{x'z'} + \epsilon_{y'y'}}{3\sqrt{2}} & \Xi_{cv} \frac{\epsilon_{y'z'} + i\epsilon_{x'z'}}{\sqrt{2}}
\end{pmatrix}
\]

where \( \Xi_{cv} \) and \( \Xi'_{cv} \) are the inter-band deformation potentials. Note that \( \Xi_{cv} \) and \( \Xi'_{cv} \) vanish in centrosymmetric crystals. The values of \( \Xi_{cv} \) and \( \Xi'_{cv} \) for HgTe and CdTe are not known. We expect \( \Xi'_{cv} \) to be much smaller than \( \Xi_{cv} \) and neglect it below.

Interfaces in heterostructures introduce additional mechanisms of Bloch state coupling. In zinc-blende structures, interface inversion asymmetry related to the anisotropy of chemical bonds leads to light-hole–heavy-hole mixing. For an arbitrary crystallographic orientation of the interface, the mixing can be described by the Hamiltonian

\[
\mathcal{H}_{68}^{\text{int}} = \frac{\hbar^2 t_{1-h}}{3a_0 m_0} \delta (\mathbf{r} \cdot \mathbf{n} + r_{\text{int}}) \sum_i \{ J_i J_{i+1} \} s n_{i+2} ,
\]

where \( t_{1-h} \) is a dimensionless mixing parameter, \( a_0 \) is the lattice constant, \( \mathbf{n} = (n_x, n_y, n_z) \) is the unit vector directed along the interface normal, say from CdHgTe to HgTe, \( r \cdot \mathbf{n} + r_{\text{int}} = 0 \) is the equation of the interface plane, and \( r_{\text{int}} \) is the distance between the interface and the coordinate origin.

To describe the electron and hole states in \((0h)\)-oriented QWs we rotate the Hamiltonian \cite{12} in the reference frame relevant to the QW. The transition from the reference frame \((x', y', z')\) to \((x, y, z)\) corresponds to the rotation around the \( x \) axis by the angle \( \theta \). Under this rotation, the basis functions \( |\Gamma_6, m\rangle \) and \( |\Gamma_8, m\rangle \) transform as the basis functions of the 1/2 and 3/2 angular momentum, respectively. Therefore, the 6-band Hamiltonian \cite{12} in the QW reference frame assumes the form

\[
\mathcal{H}_{xyz} = R^{-1} \mathcal{H} R ,
\]

where

\[
R = \begin{pmatrix}
R_6 & 0 \\
0 & R_8
\end{pmatrix} ,
\]

\( R_6 = \exp(is_x \theta) \) and \( R_8 = \exp(iJ_x \theta) \) are the \( 2 \times 2 \) and \( 4 \times 4 \) rotation matrices, respectively, and \( s_x = \sigma_x/2 \). The wave vector and strain tensor components are transformed as

\[
\begin{align*}
k_{x'} &= k_x , \\
k_{y'} &= k_y \cos \theta + k_z \sin \theta , \\
k_{z'} &= k_z \cos \theta - k_y \sin \theta ,
\end{align*}
\]

and

\[
\begin{align*}
\epsilon_{x'z'} &= \epsilon_{xx} , \\
\epsilon_{x'y'} &= \epsilon_{xy} \cos \theta + \epsilon_{xz} \sin \theta , \\
\epsilon_{x'z'} &= \epsilon_{xx} \cos \theta - \epsilon_{xz} \sin \theta , \\
\epsilon_{y'y'} &= \epsilon_{yy} \cos^2 \theta + \epsilon_{zz} \sin^2 \theta + \epsilon_{yz} \sin 2\theta , \\
\epsilon_{y'z'} &= \epsilon_{yz} \cos 2\theta + (1/2)(\epsilon_{zz} - \epsilon_{yy}) \sin 2\theta , \\
\epsilon_{z'z'} &= \epsilon_{zz} \cos^2 \theta + \epsilon_{yy} \sin^2 \theta - \epsilon_{yz} \sin 2\theta .
\end{align*}
\]

We assume that the strain in the QW is caused by mismatch between the lattice constant \( a \) of the buffer layer and the lattice constant \( a_0 \) of the unstrained QW material. Then, the in-plane strain in the QW is determined from the lattice matching condition and given by \( \epsilon_{xx} = \epsilon_{yy} = a/a_0 - 1 \). The other strain components are found from the elastic energy minimization and given by \cite{19}
where \( c_{11}, c_{12}, \) and \( c_{44} \) are the elastic constants. Note that \( c_{11} - c_{12} - 2c_{44} = 0 \) in the model of isotropic elastic medium and, hence, \( \epsilon_{yz} \neq 0 \) due to cubic shape of the unit cell.

\[
\begin{align*}
\epsilon_{zz} &= \frac{c_{11}^2 + 2c_{11}(c_{12} - c_{44}) + c_{12}(-3c_{12} + 10c_{44}) - (c_{11} + 3c_{12})(c_{11} - c_{12} - 2c_{44}) \cos 4\theta}{-c_{11}^2 - 6c_{11}c_{44} + c_{12}(c_{12} - 2c_{44}) + (c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44}) \cos 4\theta} \epsilon_{xx}, \\
\epsilon_{yx} &= \frac{\epsilon_{yx}}{c_{11}^2 - 6c_{11}c_{44} + c_{12}(c_{12} - 2c_{44}) + (c_{11} + c_{12})(c_{11} - c_{12} - 2c_{44}) \cos 4\theta} \epsilon_{xx}, \quad \epsilon_{xz} = 0, \quad \epsilon_{xy} = 0,
\end{align*}
\]

Figure 5 shows cross sections of the energy spectrum calculated numerically for asymmetric (013)-grown HgTe/Cd\(_{0.7}\)Hg\(_{0.3}\)Te QW of critical thickness. Splitting of Dirac states at \( k = 0 \) and the in-plane anisotropy of the energy spectrum are readily seen.

To obtain the parameters of the effective Hamiltonian \( \mathcal{H}^{(\text{iso})} \) we solve the Schrödinger equation \( \mathcal{H}^{(\text{xyz})} \Psi = E \Psi \) for zero in-plane wave vector, where \( \mathcal{H}^{(\text{xyz})} \) is the isotropic part of the Hamiltonian \( \mathcal{H}^{(\text{xyz})} \), and find the functions \( |E_1, \pm 1/2 \rangle \) and \( |H_1, \pm 3/2 \rangle \). Then, we project the Hamiltonian \( \mathcal{H}^{(\text{xyz})} \) onto the basis states \( |E_1, \pm 1/2 \rangle \) and \( |H_1, \pm 3/2 \rangle \). This procedure yields the effective Hamiltonian \( \mathcal{H}^{(\text{iso})} \) with \( A = P/\sqrt{2} \int f_1(z)f_3(z)dz \),

\[
\eta = \frac{\hbar^2 l_1^2}{2m_0a_0} [f_3(w/2)f_4(w/2) - f_3(-w/2)f_4(-w/2)]
\]

where \( w \) is the QW thickness and the strain tensor \( \epsilon \) is given by Eq. (24). The strain induced contributions to
Finally, we estimate the coupling parameters $\gamma$, $\eta$, $\zeta$, and $\chi$ for HgTe/Cd$_{0.7}$Hg$_{0.3}$Te QWs with the thickness $w = 6.7$ nm using the band parameters, elastic constants, and interface mixing from Refs. [21,29]. The estimation shows that the dominant contribution to $\gamma$ and $\eta$ of approximately 5 meV comes from IIA with $\eta_{1,2} \sim 1$. The strain contribution to $\eta$ is of the order of 1 meV for the interband deformation potential $\Xi_{cv} \approx -1$ eV and the strain tensor components $\epsilon_{xy} = 3 \cdot 10^{-3}$, $\epsilon_{xz} = -4 \cdot 10^{-3}$ and $\epsilon_{yz} = 10^{-3}$ calculated after Eq. (24). The BIA contribution to $\eta$ is $\sim 0.2$ meV for the parameter $B_1 \approx 0.4k^2/m_0$ estimated following Tab. 1 for $E' = 4.5$ eV [36], $Q = P$, and $P' = 0.1 P$. The $\chi$ and $\zeta$ parameters are related to SIA and estimated for the electric field $E_z = 15$ kV/cm. The contribution to $\chi$ and $\zeta$ from the cubic warping of the energy spectrum determined by $\gamma_2 - \gamma_3$ is of the order of 0.1 meV. The strain contributions to $\chi$ and $\zeta$ are about $-0.1$ meV and $-0.2$ meV, respectively. Note that SIA-related coupling parameters scale with the electric field $E_z$ and can be larger.

IV. SUMMARY

To summarize, we have studied theoretically the fine structure of Dirac states in HgTe/CdHgTe QWs of critical and close-to-critical thicknesses. Taking into account bulk, interface, and structure inversion asymmetry in these zinc-blende-type QWs, we have derived the effective Hamiltonian that describes the splitting of Dirac states in the class of (0lh)-oriented QWs from a unified standpoint. The Hamiltonian contains four parameters of splitting at zero in-plane wave vector. We have calculated these parameters in the 6-band extended Kane model, which takes into account the lack of inversion center and the cubic shape of the host crystal lattice, the elastic strain in the QW, and the heavy-hole–light-hole mixing at the QW interfaces. Further, we have derived an analytical expression for the energy spectrum of the Dirac states as a function of the growth direction and studied how the spectrum evolves from (001)- to (013)- and (011)-grown QWs. In general case, the spectrum is anisotropic and in the QWs of critical thickness contains four Weyl points. The positions of the Weyl points depend on the QW crystallographic orientation and structure inversion asymmetry and can be controlled by an external electric field applied along the QW normal, e.g., by gate voltage.

ACKNOWLEDGMENTS

This work was supported by the Russian Science Foundation (project 22-12-00211). G.V.B. acknowledges the support from the “BASIS” foundation.

1 X.-L. Qi and S. C. Zhang, Topological insulators and superconductors, Rev. Mod. Phys. 83, 1057 (2011).
2 Z. D. Kvon, D. A. Kozlov, E. B. Olshanetsky, G. M. Gusev, N. N. Mikhailov, and S A Dvoretsky, Topological insulators based on HgTe, Phys.-Uspek. 63, 629 (2020).
3 B. Büttnner, C. X. Liu, G. Tkachov, E. G. Novik, C. Brüne, H. Buhmann, E. M. Hankiewicz, P. Recher, B. Trauzettel, S. C. Zhang, and L. W. Molenkamp, Single valley Dirac fermions in zero-gap HgTe quantum wells, Nat. Phys. 7, 418 (2011).
4 S. A. Tarasenko, M. V. Durnev, M. O. Nestoklon, E. L. Ivchenko, J.-W. Luo, and A. Zunger, Split Dirac cones in HgTe/CdTe quantum wells due to symmetry-enforced level anticrossing at interfaces, Phys. Rev. B 91, 081302(R) (2015).
5 X. Dai, T. L. Hughes, X. L. Qi, Z. Fang, and S. C. Zhang, Helical edge and surface states in HgTe quantum wells and bulk insulators, Phys. Rev. B 77, 125319 (2008).
6 M. König, H. Buhmann, L.W. Molenkamp, T. L. Hughes, C.-X. Liu, X. L. Qi, and S. C. Zhang, The quantum spin Hall effect: theory and experiment, J. Phys. Soc. Jpn. 77, 031007 (2008).
7 R. Winkler, L. Y. Wang, Y. H. Lin, and C. S. Chu, Robust level coincidences in the subband structure of quasi-2D systems, Solid State Commun. 152, 2096 (2012).
8 L. Weithofer and P. Recher, Chiral Majorana edge states in HgTe quantum wells, New J. Phys. 15, 085008 (2013).
9 M. Orlita, K. Masztalerz, C. Faugeras, M. Potemski, E. G. Novik, C. Brüne, H. Buhmann, and L. W. Molenkamp, Fine structure of zero-mode Landau levels in HgTe/Hg$_{1-x}$Cd$_x$Te quantum wells, Phys. Rev. B 83, 115307 (2011).
10 M. Zhohudev, F. Teppe, M. Orlita, C. Consejo, J. Torres, N. Dyakonova, M. Czapkiewicz, J. Wróbel, G. Grabecì, N. Mikhailov, S. Dvoretskyi, A. Ikonnikov, K. Spirim, V. Aleshkin, V. Gavrilko, and W. Knap, Magnetospectroscopy of two-dimensional HgTe-based topological insulators around the critical thickness, Phys. Rev. B 86, 205420 (2012).
11 P. Olbrich, C. Zoth, P. Vierling, K.-M. Dantscher, G. V. Budkin, S. A. Tarasenko, V. V. Belkov, D. A. Kozlov, Z. D. Kvon, N. N. Mikhailov, S. A. Dvoretsky, and S. D. Ganichev, Giant photocurrents in a Dirac fermion system at cyclotron resonance, Phys. Rev. B 87, 235439 (2013).
12 G. M. Minkov, A.V. Germanenko, O. E. Rut, A. A. Sherstobitov, M. O. Nestoklon, S. A. Dvoretsky, and N. N. Mikhailov, Spin-orbit splitting of valence and conduction bands in HgTe quantum wells near the Dirac point, Phys. Rev. B 93, 155304 (2016).
13 M. V. Durnev and S. A. Tarasenko, Magnetic field effects on edge and bulk states in topological insulators based on HgTe/CdHgTe quantum wells with strong natural interface inversion asymmetry, Phys. Rev. B 93, 075434 (2016).
14 E. I. Rashba, Properties of semiconductors with an extremum loop. 1. Cyclotron and combinational resonance in a magnetic field perpendicular to the plane of the loop, Sov.
Phys. Solid. State 2, 1109 (1960).

15. F. T. Vasko, Spin splitting in the spectrum of two-dimensional electrons due to the surface potential, JETP Lett. 30, 541 (1979).

16. Y. A. Bychkov and E. I. Rashba, Properties of a 2D electron gas with lifted spectral degeneracy, JETP Lett. 39, 78 (1984).

17. G. Dresselhaus, Spin-orbit coupling effects in zinc blende structures, Phys. Rev. 100, 580 (1955).

18. M. I. D’yakonov and V. Y. Kachorovskii, Spin relaxation of conduction electrons in noncentrosymmetric semiconductors, Sov. Phys. Semicond. 20, 110 (1986).

19. G. E. Pikus, V. A. Maruschak, and A. N. Titkov, Spin splitting of energy bands and spin relaxation of carriers in cubic III-V crystals, Sov. Phys. Semicond. 22, 115 (1988).

20. E. I. Rashba and E. Y. Sherman, Spin-orbital band splitting in symmetric quantum wells, Phys. Lett. A 129, 175 (1988).

21. K.-M. Dantscher, D. A. Kozlov, P. Olbrich, C. Zoth, P. Faltermeyer, M. Lindner, G. V. Budkin, S. A. Tarasenko, V. V. Bel’kov, Z.D. Kvon, N. N. Mikhailov, S. A. Dvoretsky, D. Weiss, B. Jenichen, and S. D. Ganichev, Cyclotron-resonance-assisted photocurrents in surface states of a three-dimensional topological insulator based on a strained high-mobility HgTe film, Phys. Rev. B 92, 165314 (2015).

22. K.-M. Dantscher, D. A. Kozlov, M. T. Scherr, S. Gebert, J. Bärendänger, M. V. Durnev, S. A. Tarasenko, V. V. Bel’kov, N. N. Mikhailov, S. A. Dvoretsky, Z. D. Kvon, J. Ziegler, D. Weiss, and S. D. Ganichev, Photogalvanic probing of helical edge channels in two-dimensional HgTe topological insulators, Phys. Rev. B 95, 201103(R) (2017).

23. G. M. Minkov, V. Ya. Aleshkin, O. E. Rut, A. A. Sherstobitov, A. V. Germanenko, S. A. Dvoretsky, and N. N. Mikhailov, Valence band energy spectrum of HgTe quantum wells with an inverted band structure, Phys. Rev. B 96, 035310 (2017).

24. S. Dvoretsky, N. Mikhailov, D. Ikusov, V. Kartashev, A. Kolesnikov, I. Sabinina, Y. G. Sidorov, and V. Shvets, The growth of CdTe layer on GaAs substrate by MBE, in Methods for Film Synthesis and Coating Procedures (IntechOpen, 2020).

25. O. E. Raichev, Effective Hamiltonian, energy spectrum, and phase transition induced by in-plane magnetic field in symmetric HgTe quantum wells, Phys. Rev. B 85, 045310 (2012).

26. G. V. Budkin and S. A. Tarasenko, Spin splitting in low-symmetry quantum wells beyond Rashba and Dresselhaus terms, Phys. Rev. B 105, L161301 (2022).

27. B. A. Bernevig, T. L. Hughes, and S.-C. Zhang, Quantum Hall effect and topological phase transition in HgTe quantum wells, Science 314, 1757 (2006).

28. L. G. Gerchikov and A. V. Subashiev, Non-monotonic behavior of the energy gap in the film made of a gapless semiconductor, Sov. Phys. Semicond. 23, 1368 (1989).

29. E. G. Novik, A. Pfeuffer-Jeschke, T. Jungwirth, V. Latyshev, C. R. Becker, G. Landwehr, H. Buhmann, and L. W. Molenkamp, Band structure of semimagnetic Hg$_{1-y}$Mn$_y$Te quantum wells, Phys. Rev. B 72, 035321 (2005).

30. R. Winkler, Spin-Orbit Coupling Effects in Two-Dimensional Electron and Hole Systems, (2003).

31. G. L. Bir and G. E. Pikus, Symmetry and Strain-induced Effects in Semiconductors, (Wiley, New York, 1974).

32. J.-M. Jancu, R. Scholz, E. A. de Andrade e Silva, and G. C. L. Rocca, Atomistic spin-orbit coupling and $kp$ parameters in III–V semiconductors, Phys. Rev. B 72, 193201 (2005).

33. M. V. Durnev, M. M. Glazov, and E. L. Ivchenko, Spin-orbit splitting of valence subbands in semiconductor nanostructures, Phys. Rev. B 89, 075430 (2014).

34. I. L. Aleiner and E. L. Ivchenko, Anistropic exchange splitting in type II GaAs/AlAs superlattices, JETP Lett. 55, 692 (1992).

35. E. L. Ivchenko, A. Y. Kaminski, and U. Rössler, Heavy-light hole mixing at zinc-blende (001) interfaces under normal incidence, Phys. Rev. B 54, 5852 (1996).

36. Z. W. Lu, D. Singh, and H. Krakauer, Total-energy study of the equation of state of HgTe and HgSe, Phys. Rev. B 39, 10154 (1989).