Fine structure of “zero-mode” Landau levels in HgTe/HgCdTe quantum wells

M. Orlita,1,† K. Masztalerz,1,‡ C. Faugeras,1 M. Potemski,1
E. G. Novik,2 C. Brüne,2 H. Buhmann,2 and L. W. Molenkamp2

1Laboratoire National des Champs Magnétiques Intenses,
CNRS-UF-UPS-INSA, 25, avenue des Martyrs, 38042 Grenoble, France
2Physikalisches Institut (Lehrstuhl für Experimentalphysik III),
Universität Würzburg, D-97074, Würzburg, Germany

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HgTe/HgCdTe quantum wells with the inverted band structure have been probed using far infrared magneto-spectroscopy. Realistic calculations of Landau level diagrams have been performed to identify the observed transitions. Investigations have been greatly focused on the magnetic field dependence of the peculiar pair of “zero-mode” Landau levels which characteristically split from the upper conduction and bottom valence bands, and merge under the applied magnetic field. The observed avoided crossing of these levels is tentatively attributed to the bulk inversion asymmetry of zinc blend compounds.

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I. INTRODUCTION

Experimental finding of the quantum spin Hall effect (QSHE) in HgTe/CdTe quantum wells (QWs) affirmed the previous theoretical predictions and has had a relevant impact on further development of the research on two- and three-dimensional (2D and 3D) topological insulators. Remarkably, the origin of the topological insulator phase (bulk gapped insulator with gapless conducting states at the edges or surfaces) turns out to be just the peculiar band structure, characteristic of certain class of semiconductors with an appropriate strength of spin-orbit interaction.

The 2D archetype of this phase appears in HgTe quantum wells in the regime of the so-called inverted band structure (semiconductor with a gap between the upper p-type and lower s-type energy band). The inherent property of such bands is their characteristic behavior under the applied magnetic field, i.e., the appearance of the particular pair of Landau levels (LLs) which distinctly split from the upper and lower energy band. Progressively with the magnetic field, those two Landau levels merge and eventually cross at a critical field \(B_c\), above which the zero-field topologically insulating phase is transformed into the common quantum Hall insulator.

The origin of this distinct pair of LLs and its possible interesting physics becomes apparent when using a modified \(4 \times 4\) Dirac-type Hamiltonian for the approximate description of the Fermi level-vicinity electronic states. In case of HgTe QWs, the off-diagonal terms of the massless Dirac Hamiltonian have to be completed by the diagonal (dispersive) mass terms. Nevertheless, the above-mention particular pair of Landau levels still appears due to the off-diagonal, linear in particle momentum terms. It is a reminiscence of the characteristic, field-independent zero-mode (zero-index) Landau levels of massless Dirac fermions, such as, for example, those found in graphene. In HgTe QWs, these levels are split in energy due to the mass term and their positions change monotonically as a function of the width of the quantum well. In case of inverted bands, this splitting becomes negative what intuitively accounts for merging of zero-mode LLs in a magnetic field. Notably, the zero-mode Landau levels in HgTe are spin polarized (even if the bare Zeeman splitting is ignored) similarly like the zero-mode levels are pseudo-spin polarized in graphene, i.e., with charge localized on either of two triangular sublattices.

As reported before, the magnetic field evolution of the zero-mode LLs in HgTe QWs with the inverted band structure is at the origin of the field-driven insulator-metal-insulator phase transition, characteristic of these systems. A simple scenario of crossing of those levels at a critical field \(B_c\) has been sufficient to account for the magneto-transport data, but a possibility of a weak anti-crossing effect has also been considered.

In this paper, we inspect more closely the field evolution of these “zero-mode” Landau levels using a suitable experimental tool of Landau level spectroscopy. Essentially, we find that the zero-mode Landau levels in HgTe quantum wells with the inverted band structure do not cross, but instead display the effect of the avoided crossing. This effect might be due to the bulk inversion asymmetry (BIA) which is inherently present in zinc-blend crystals but habitually neglected in band structure calculations of HgTe quantum wells. A more speculative interpretation of our experimental finding would consist of refereeing to the extended investigations of the zero-mode Landau levels in graphene and pointing out the electron-electron interaction as a possible source of opening of a gap within the otherwise double degenerate Landau level at the critical field \(B_c\).

II. EXPERIMENTAL DETAILS

We have studied two different samples, each containing a 8 nm-wide, [001]-oriented HgTe quantum well embedded in-between \(\text{Hg}_{0.3}\text{Cd}_{0.7}\text{Te}\) barriers. The band struc-
ture of QWs in both samples is inverted. Since we work with relatively narrow QWs, the first electron-like subband ($E_1$) is above the second heavy-hole subband (HH$_2$). This is in contrast to the case of structures used in previous magneto-optical studies$^{13,14}$ The sample denoted here as $A$ was intentionally undoped but its residual $p$- or $n$-doping at the level up to $10^{11}$ cm$^{-2}$ is not excluded. The QW in the sample B was symmetrically doped with iodium donors, separated from the well by 40 nm-wide barrier spacers. The density of 2D electron gas (2DEG), $n = 4.2 \times 10^{11}$ cm$^{-2}$, has been determined from magneto-transport measurements on a parent sample (not discussed in this paper). This value served us as an input parameter for calculations of the band structure and the resulting energy ladder of LLs in this sample.

To measure the infrared transmittance, the sample was exposed to the radiation of a globar, which was analyzed by a Fourier transform spectrometer and delivered to the sample via light-pipe optics. The transmitted light was detected by a composite bolometer which operated at $T = 2$ K and was placed directly below the sample. The magneto-optical spectra were measured using either a superconducting coil ($B \leq 13$ T, applied spectral resolution of 0.5 meV) or a resistive solenoid (magnetic fields up to 30 T, applied spectral resolution of 1 meV). All the spectra presented here were normalized by the sample transmission at $B = 0$.

III. LANDAU LEVEL SPECTRUM IN HGTE/HGCDTE QUANTUM WELLS

The detailed LL spectrum of HgTe/HgCdTe QWs is in general derived from the Kane’s band structure model and the resulting $8 \times 8$ Hamiltonian.$^{12,15}$ This, at $B > 0$, implies solving a set of eight coupled differential equations for a given LL index $N$, which results in eight independent solutions for $N > 0$ (four pairs of spin-split LLs). Importantly, only 7, 4 and 1 non-trivial solutions are obtained for low indices $N = 0, -1$ and -2, respectively. A single, $N = -2$ LL has a purely heavy-hole character ($S = -3/2$) and its energy decreases nearly linearly with $B$. This level together with one of the characteristic solutions for $N = 0$ represent our zero-mode LLs which we have identified within a simplified approach of the Dirac-type Hamiltonian in the introductory part of this paper.

In calculations of LL diagrams of our two QW structures, we have applied a general scheme of the Kane model but neglected the BIA effect. Such an approximation implies that, for any QW structure in the inverted regime, the two zero-mode LLs (or the characteristic $N = -2$ and $N = 0$ LLs) simply cross each other at a given (well width dependent) magnetic field $B_c$. These characteristic levels and their crossing can be easily recognized in Fig. 4 for the case of our samples.

Figure 1 illustrates the details of our LL calculations in the relevant energy range of the proximity of the $E_1$, HH$_1$ and HH$_2$ subbands and depicts the transitions which are expected to be observed in the experiment. Optically active inter-LL transitions follow the usual $\Delta N = \pm 1$ (for $\sigma^\pm$ circularly polarized light) selection rules imposed by the electric dipole approximation. The oscillator strength of the transitions depends also on the overlap of LL wavefunction in the $z$-direction, what is, however, not essential for the present considerations. Concluding the previous studies of HgTe QWs,$^{13,14}$ we expect the magneto-optical response of our structures to be dominated by transi-
tions between LLs with low indices. Those transitions are marked in Fig. 1 with small Greek letters, in accordance to the notation of Schultz et al. Transition $\alpha$ accounts for the expected dominant interband LL transition whereas $\beta$, $\gamma$ and $\delta$ denote the cyclotron resonance (CR) like transitions between the adjacent LLs of the same (HH$_1$) subband.

IV. RESULTS AND DISCUSSION

Typical transmission spectra measured at a few selected values of the magnetic field are plotted in Fig. 2. The corresponding, energy versus magnetic field LL diagrams of the observed transitions are shown in Fig. 3. Inspection of the calculated diagrams (see Fig. 1) and the results of previous studies of similar structures provides an important input to the assignment of the measured absorption lines.

Sample B shows a single absorption line at low magnetic fields. This line can be identified as a cyclotron resonance absorption due to 2DEG confined in the QW, see Figs. 1b, 2b and 3b. The CR-like absorption is at low fields nearly linear with $B$ and implies $m^* = 0.022m_0$ for the carrier effective mass at the Fermi level. Characteristically for narrow-gap materials with strongly non-parabolic bands, the CR energy versus $B$ dependence appears to be sub-linear at higher fields. Once the CR line emerges above the reststrahlen band of HgTe/HgCdTe, it corresponds to inter-LL transition $\delta$ (HH$_1$: $N = 1 \rightarrow$ HH$_1$: $N = 2$). Around $B \approx 7$ T, the $\gamma$ line (HH$_2$: $N = -1 \rightarrow$ HH$_1$: $N = 0$) appears in the spectrum and it gains in intensity at the expense of the $\delta$ line. At even higher fields, the $\gamma$ line weakens and finally disappears from the spectrum at $B \approx 17$ T. Assuming that $B = 17$ T corresponds to the Landau level filling factor $\nu = 1$, we find an excellent agreement upon the density of the 2DEG, which has been derived from magneto-transport measurements on a parent sample. Consistently, the $\alpha$ line (E$_1$: $N = 0 \rightarrow$ HH$_1$: $N = 1$) appears in the spectrum around $B \approx 6$ T, i.e. for $\nu \leq 3$, and reaches its maximum intensity for $\nu = 2$ at $B \approx 12$ T. Its oscillator strength starts to gradually decrease once filling factor decreases below $\nu = 1$.

The exact level of doping in sample A is unknown and therefore the analysis of the magneto-absorption data of this sample is more difficult. The appearance of the $\alpha$ transition is nevertheless clear. This line is a common feature observed in both samples and its energy position correlates well with the results of calculations. In sample A, the $\alpha$ line remains visible in the spectra up to magnetic fields of $B \approx 13$ T, which points towards the residual $n$-type doping of this QW structure. This doping level is however low, thus no CR-like transitions are seen. The identification of the second line visible in the spectra of sample A is a more subtle issue. Very likely, this line is associated with the transition HH$_1$: $N = -2 \rightarrow$ HH$_1$: $N = -1$, i.e. with the $\beta$ transition of Fig. 1. Nevertheless, the measured spectral position of this line somewhat deviates from the theoretical expectation and therefore we cannot exclude that it also involves some over transitions which originate from LLs of the E$_1$ and/or HH$_2$ subbands. In addition, the exact spectral shape of this line is masked by the overlapping extra feature (appearing in both sample at $\approx 50$ meV) due to acceptor states in CdTe substrate. Notably, in sample B, the $\beta$ transition is blocked at low magnetic fields by $n$-type doping but surprisingly it does not appear in the spectra at high magnetic fields $B > 8$ T when $\nu < 2$, i.e., when the final-state LL associated with this transition is emptying. We may speculate that the oscillator strength of the $\beta$ line is reduced at high magnetic fields due to merging of the $N = -2$ LL with the quasi-continuum of valence band LLs (see Fig. 1).

Obviously, the above approach to interpreted the data does not take into account all possible effects which may influence the measured spectra. Among those are the effects of bulk inversion symmetry and electron-electron interactions. Notably, these latter effects may also largely influence the energies and degeneracy of inter Landau transitions as we deal with strongly non-parabolic systems for which Kohn’s theorem does not hold.

FIG. 3: (color online) Fanchart of inter-LL transitions in both investigated samples. Solid lines show the expected single-particle excitation energies following the calculation presented in Fig. 1. In both samples, the experimentally traced $\alpha$ transition shows a double component character in the vicinity of the crossing fields $B_c$. The dashed lines represent the expected position of the $\alpha$ transition taking account the mixing of $N = 0$ and $-2$ Landau levels, calculated according to König et al. for the phenomenological coupling parameter $\Delta = 2$ meV.
In the following, our attention is focused on the α transition which is an unambiguously defined spectral feature observed in both investigated samples and involves the $N = 0$ zero-mode LL in the initial state. As can be seen in Fig. 4 the α line has a character of a doublet visible in the spectra in a relatively narrow range of magnetic fields, $B = 6 − 8$ T. Exactly in this field interval, at $B ≈ 7$ T, the crossing of the zero mode, $N = 0$ and $N = −2$, LLs is inferred from our calculations (see Fig.1B). Instead, the observation of the doublet structure indicates that those two LLs are never degenerate. Level anti-crossing is one possible scenario to account for this experimental fact.

To model such an effect we have followed a standard perturbation approach and phenomenologically hybridized the initially calculated uncoupled $N = 0$ and $N = −2$ LLs. The avoided crossing of the resulting coupled modes is shown with dashed lines in Fig.3. Assuming $Δ = 2 \text{ meV}$ for the coupling parameter we roughly reproduce the observed $\approx 4 \text{ meV} (= 2Δ)$ energy separation between the doublet components of the α line in the sample A. Doublet splitting seems to be slightly smaller in the sample A. We note, however, that the appearance of the doublet structure in sample B is pretty abrupt whereas our simple anti-crossing model would imply that this doublet persists in somewhat wider range of magnetic fields. As discussed by König et al., the hybridization of heavy-hole-like $\Gamma_8$ and $\Gamma_6$ states with opposite spin direction and therefore coupling between the $N = 0$ and $N = −2$ LLs may results from the breaking of bulk inversion symmetry, initially neglected in our calculations. The theoretically estimated amplitude of coupling parameter imposed by the BIA terms reaches $Δ \sim 1.6 \text{ meV}$ in structures similar to ours.

Optionally, we speculate that the observed splitting of the otherwise degenerate zero mode LLs at the critical field $B_c$ might be also induced by electron-electron interactions. We note that physics of our zero-Landau level in the vicinity of $B_c$ might be similar to that of a widely discussed case of the $n = 0$ Landau level in graphene. The degeneracy of this latter level is indeed believed to be lifted by electron-electron interactions due to, for example, spontaneous spin polarization. Independently of its origin, the persistent splitting between our zero mode LLs may have a relevant consequences on the detailed nature of the magnetic field driven insulator-metal-insulator transition. For example, the metallic phase might be absent in this transition if the system is kept as perfectly neutral. The accurate determination of the BIA terms may also help to uncover more details of the QSHE, for example, in reference to its quenching by the application of the perpendicular magnetic field.

V. CONCLUSIONS

We have explored the fine structure of Landau levels in [001]-oriented HgTe/HgCdTe quantum wells with an inverted band structure using infrared magneto-spectroscopy. Our particular attention has been focused on the low-lying conduction band and top-most valence band Landau levels, i.e. on the zero-mode levels of this Dirac-type system. We have found a spectroscopic signature of avoided crossing (splitting at critical field $B_c$) of these levels. This effect is likely due to the breaking of bulk inversion symmetry, but perhaps also mediated by electron-electron interactions. Our experimental findings may have a relevant consequences on the subtleties of the physics of QSHE and magnetic-field-driven insulator-metal-insulator, the two characteristic and intriguing phenomena observed in HgTe structures.

Acknowledgments

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