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Article

Experimental Observation of Temperature-Driven Topological Phase Transition in HgTe/CdHgTe Quantum Wells

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Abstract: We report on comparison between temperature-dependent magnetoabsorption and magnetotransport spectroscopy of HgTe/CdHgTe quantum wells in terms of detection of phase transition between topological insulator and band insulator states. Our results demonstrate that temperature-dependent magnetospectroscopy is a powerful tool to discriminate trivial and topological insulator phases, yet magnetotransport method is shown to have advantages for clear manifestation of the phase transition with accurate quantitative values of transition parameter (i.e. critical magnetic field B_c).

Keywords: topological insulator; phase transition; mercury cadmium telluride; Landau levels; magnetoabsorption; magnetotransport

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1. Introduction

Due to their amazing electronic properties, 2D and 3D topological insulators (TI) have attracted increasing attention within the last decade. Simultaneously, HgTe/CdHgTe quantum well (QW) was the first system where the TI state was predicted [1] and experimentally observed [2]. The inversion of electron-like level E1 and hole-like level H1 induces spin-polarized helical edge states [2]. When E1 and H1 levels cross each other, the band structure mimics a linear dispersion of massless Dirac fermions [3] corresponding to the phase transition between trivial band insulator (BI) and TI states.

By fabricating QWs with different thicknesses, the band structure can be widely tuned, i.e. it is inverted if QW thickness d exceeds the critical value d_c = 6.3 nm for HgTe/$Cd_{0.7}Hg_{0.3}$Te QWs grown on CdTe buffer, whereas the band structure is normal for $d < d_c$ [1]. At the critical thickness, the band gap closes, establishing single-valley 2D massless Dirac fermions [3].

In addition to the QW thickness, temperature [4,5] and hydrostatic pressure [6] also induces the transition between BI and TI phases across the critical gapless state. The temperature effect on the band ordering in HgTe/CdHgTe QWs is mainly caused by a strong temperature dependence of the energy gap at the Γ point of the Brillouin zone between the Γ6 and Γ8 bands in HgCdTe crystals [7]. In the essence temperature changes (decreases) the critical thickness of HgTe/CdHgTe QWs. The point where the critical thickness is equal to the actual size of the well is the critical temperature T_c.

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Any phase transition implies discontinuous change of some parameter, e.g. specific volume (melting, boiling) or first derivative of order parameter (ferromagnetic, superconductors). Order parameter concerning edge states of TI phase can be introduced in theory but it is hardly useful in practice because detection of these states is very difficult. Fortunately; there are other parameters that change abruptly between TI and BI phases and can be experimentally measured. The first one is the energy gap temperature dependence that has negative derivative below the critical point and positive derivative above it. The main flaw of direct band gap measurements is that observation of small energy gap by light absorption or transmission is very difficult even at liquid helium temperatures and impossible at high temperatures.

Another possible approach is based on the analysis of the behavior of Landau levels (LLs) in high magnetic fields. Figure 1 illustrates typical LL pictures for BI, zero-gap and TI cases with the transitions that are usually observed in magnetoabsorption experiments. One of the inherent properties of inverted band HgTe/CdHgTe QWs is the behavior of zero-mode LLs with indices $N = 0$ and $N = -2$ (bold lines on Figure 1). In the BI phase these levels belong to conduction and valence bands respectively and do not cross (Figure 1a). Within QWs in the TI phase (Figure 1c), zero-mode LLs have reverse start positions (at $B = 0$) and consequently cross at a critical magnetic field B_c, above which inverted band ordering is transformed into normal one [2]. The latter can be conditionally interpreted as negative values for B_c. Thus, $B_c = 0$ corresponds to a topological phase transition between BI and TI phases. As it is for the band ordering, a critical magnetic field also depends on temperature and pressure, and therefore, can be varied by tuning these external parameters [6].

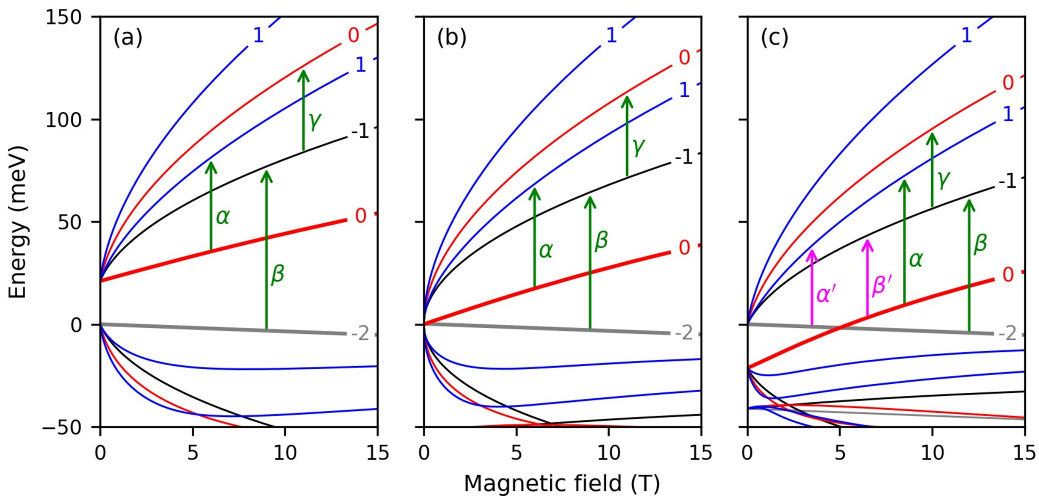

Figure 1. Landau levels of HgTe/$Cd_{0.7}Hg_{0.3}Te$ QW calculated with axial approximation for: (**a**) band insulator ($d = 5.5$ nm); (**b**) zero-gap semiconductor ($d = 6.3$ nm); (**c**) topological insulator ($d = 7.4$ nm). Zero-mode LLs are shown with bold lines. LL indices are shown with both numbers on the lines and line colors. We use the same calculation method and notation of LL indices as in [9,10].

By analyzing magnetotransport data at high and low temperatures, S. Wiedmann et al. [5] have experimentally shown that TI phase vanishes with temperature. However, due to high critical temperature Tc (above 200 K) the gapless state couldn't be directly observed in the samples studied. A.V. Ikonnikov et al. [8] have reported on magnetospectroscopy of HgTe quantum wells in magnetic fields up to 45 T in temperature range from 4.2 K up to 185 K. They show that although their samples are TI only at low temperatures, the signature of such phase persists in optical transitions at high temperatures and high magnetic fields. In our previous works we have reported on the observation of temperature driven topological phase transition by far-infrared magnetoabsorption

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spectroscopy [11] and magnetotransport [12,13]. In the present work we analyse these two methods and make a conclusion about their applicability for TI-BI phase transition investigation.

2. Results

It is clear from Figure 1a that in BI state α is an intraband transition within the conduction band and β is an interband transition. In TI state (Figure 1c) α is an interband transition and β is an intraband transition. Both α and β lines have been observed in our experiment [11] (see Figure 2). The position of interband line should give us the band gap value when followed down to zero magnetic field. Unfortunately, doing this was impossible in the framework of our experiments [11]. Instead of that in the work [11] we had to use extrapolation of experimentally observed α and β transition lines to estimate the band gap. This approach, however, is not reliable because of the specific type of functions used for extrapolation (Figure 3). For these square-root-like functions a small difference at high magnetic fields results into big difference at zero magnetic field. Hence, small error in experimental data leads to big error in the estimated energy gap. This effect is especially strong in inverted-band QWs because of the disagreement of theoretical and experimental line positions (see Figure 2f,g). Consequently we should conclude that we cannot trust the energy gap values reported in [11].

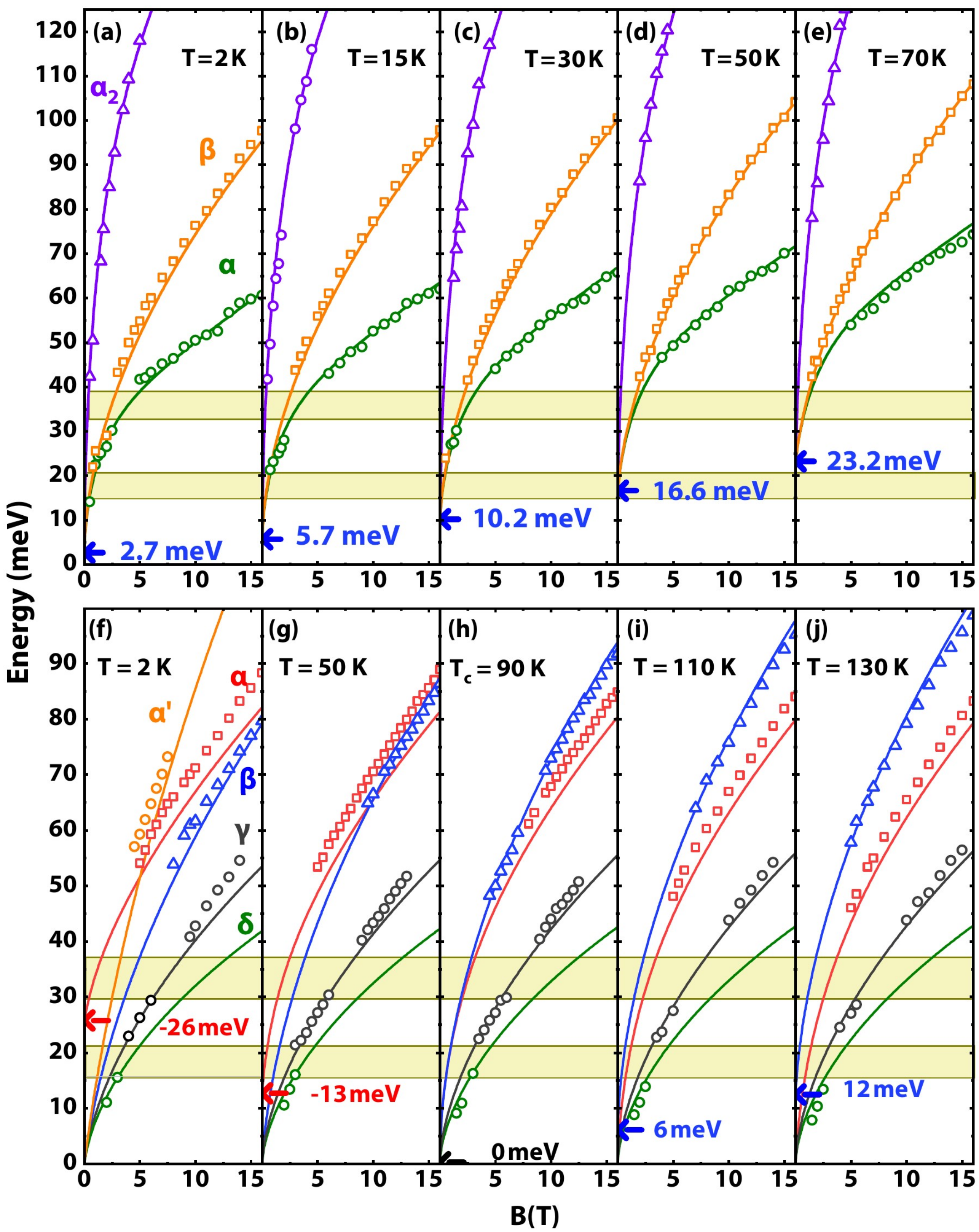

Figure 2. Fan chart of inter-LL transitions in 6 nm width HgTe/$Cd_{0.62}Hg_{0.38}Te$ QW (**a**-**e**) and 8 nm width HgTe/$Cd_{0.8}Hg_{0.2}Te$ QW (**f**-**j**) from work [11]. The calculated transitions are shown in solid lines while experimental data are represented by open symbols in the same colors as the theoretical curves. The estimated values of the energy gap are shown by horizontal arrows. Shaded areas indicate the GaAs and HgCdTe reststrahlen bands.

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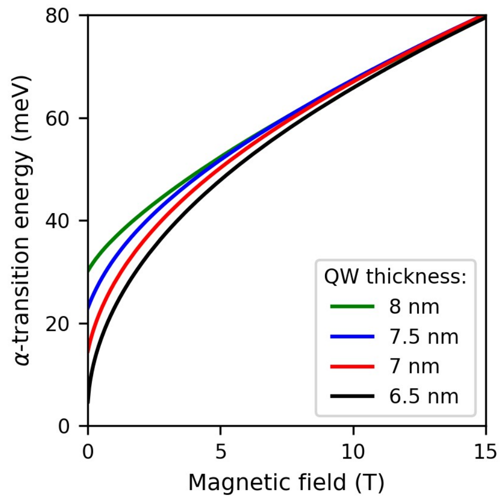

Figure 3. Calculated energy of α-transition for HgTe/$Cd_{0.7}Hg_{0.3}Te$ QWs of different thickness.

The fact of phase transition, however, can still be seen from these experimental data. For that we suggest another approach based on qualitative difference in the structure of the transition lines in TI and BI. For TI state there are two transitions α' and β' that are forbidden by selection rules in the simple model we use (see Figure 1c). The corresponding lines, however, can be observed because of mixing of the zero-mode LLs near the crossing point [9,14] (line α' is shown on Figure 2f). Hence in magnetoabsorption experiments we cannot observe the crossing of LLs directly, but can see the consequences of LL mixing (i.e. emergence of lines α' and β') and hence detect the TI state. The limitation of this method is that anticrossing can be clearly seen only when B_c is high enough so that α and β transitions are not forbidden by Pauli principle and the crossing point does not fall in the restrahlen bands (see Figure 2f). Consequently, in the vicinity of the conditions corresponding to phase transition when B_c is close to zero no manifestation of the LL anticrossing can be observed (see Figure 2g,h).

Another approach is based on analyzing behavior of α and β lines in high magnetic fields where they are clearly seen at all temperatures. In Figure 1 one can see that the energy of lower level of α transition ($N = 0$) goes up with magnetic field while the energy of lower level of β transition ($N = -2$) goes down, on the other hand, the energy of upper levels ($N = 1$ and $N = -1$) goes up for both transitions. Thus the energy of β line will always have higher derivative over magnetic field than the one of α line. Because of this in BI state β line lies above α line and never crosses it (Figure 2a-e). Our calculations show that in TI state β line starts from zero and should cross α line at some point, however, in the experiment we see two parallel lines (see e.g. Figure 2f,g). We believe that it comes from magnetic field being too weak to reach the α-β crossing point. The lines look parallel because their energies close to B_c are affected by aforementioned α-α' and β-β' anticrossing [9,14]. Hence at these conditions the behavior of α and β lines predicted by simple axial model cannot be observed due to interference with low symmetry effects around B_c and the limitation of maximal magnetic field. At critical temperature the crossing of α and β lines was observed (Figure 2h). Above the critical temperature we can clearly see that β line (that has higher slope) lies above α line as expected for BI state (Figure 2i,j).

An alternative method that allows to detect topological phase transition is based on magnetotransport measurements in gated Hall bar [13]. The ability to set the Fermi level in a wide range by applied gate voltage Vg, allows one to perform a magnetotransport mapping of the structure of LLs of our sample. As it was proposed in the pioneer paper by Büttner et al. [3], the peaks of $\partial\sigma_{xy}/\partial V_g$ curves give the precise positions of crossings between the Fermi level and the LLs.

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Therefore plotting $\partial\sigma_{xy}/\partial V_g$ for each magnetic field value makes it possible to reveal the dispersion of the LLs (see Figure 4).

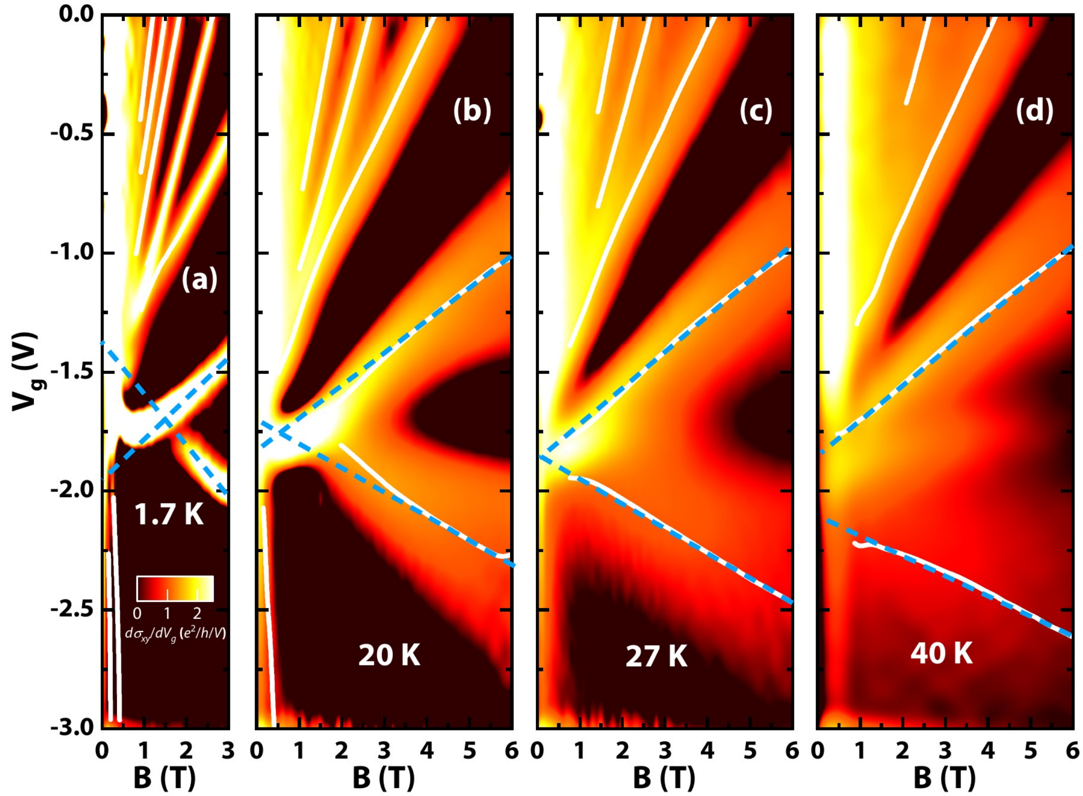

Figure 4. Colormap of the experimental Landau level fan charts of derivative $\partial\sigma_{xy}/\partial V_g$ in 6.5 nm width $HgTe/Cd_{0.65}Hg_{0.35}Te$ QW as a function of both magnetic field and gate voltage from work [13]; brighter color represents higher value of the derivative; dark color represents lower value. The white curves present positions of $\sigma_{xy} = (2n + 1)e^2/(2h)$. The blue dashed curves fit experimental behavior of the zero-mode LLs based on σ_{xy} values at high magnetic fields.

In the work [13] we define the critical magnetic field B_c as position of the crossing of zero-mode LLs or their linear extrapolation. Consequently the value of B_c can be negative that corresponds to normal semiconductor phase. It is necessary to note that extrapolation we use is much more accurate than the one used in magnetooptical experiments. The measurements have shown that when Fermi level is located within conduction or valence band the value of 2D carrier concentration depends linearly on the gate voltage V_g [15]. Consequently, as far as the LL degeneracy rate is also proportional to 2D carrier concentration, all LLs in Figure 4 are exactly linear everywhere except the range where Fermi level lies in the gap (-2 V < V_g < -1.5 V). Thus the method used in work [13] allows precise measurement of both positive and negative B_c values (see Figure 5) and is reliable instrument to probe a temperature-induced phase transition between BI and TI phases.

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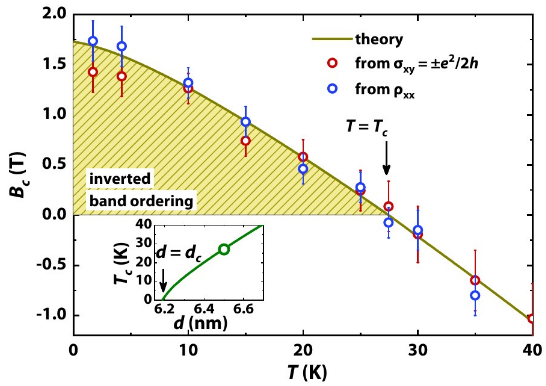

Figure 5. Theoretical (black curve) and experimental (open symbols) values for critical magnetic field as a function of temperature for 6.5 nm HgTe/$Cd_{0.65}Hg_{0.35}Te$ QW from work [13].

3. Conclusion

Magnetotransport experiments give clear manifestation of T-driven TI-BI phase transition with accurate quantitative values of transition parameter (i.e. critical magnetic field B_c). Magnetooptical experiments give only qualitative picture and any estimations of energy gap based on these measurements are inaccurate.

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Conflicts of Interest: The authors declare no conflict of interest. The funders had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, or in the decision to publish the results.

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