Double valley Dirac fermions for 3D and 2D Hg\textsubscript{1−x}Cd\textsubscript{x}Te with strong asymmetry

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Abstract – In this paper the possibility to bring about the double-valley Dirac fermions in some quantum structures is predicted. These quantum structures are: strained 3D Hg\textsubscript{1−x}Cd\textsubscript{x}Te topological insulator (TI) with strong interface inversion asymmetry and the asymmetric Hg\textsubscript{1−x}Cd\textsubscript{x}Te double quantum wells (DQW). The numerical analysis of the dispersion relation for 3D TI Hg\textsubscript{1−x}Cd\textsubscript{x}Te for the proper Cd (x)-content of the Hg\textsubscript{1−x}Cd\textsubscript{x}Te compound clearly shows that the inversion symmetry breaking together with the unaxial tensile strain causes the splitting of each of the Dirac nodes (two belonging to two interfaces) into two in the proximity of the Γ-point. Similar effects can be obtained for asymmetric Hg\textsubscript{1−x}Cd\textsubscript{x}Te DQW with the proper content of Cd and proper width of the quantum wells. The aim of this work is to explore the inversion symmetry breaking in 3D TI and 2D DQW mixed HgCdTe systems. It is shown that this symmetry breaking leads to the dependence of carriers energy on quasi-momentum similar to that of Weyl fermions.

Introduction. – In ref. [1] the existence of 3D topological insulators (TI) in the HgTe 75–80 nm wide strained layers has been predicted theoretically, and it was later confirmed experimentally in the work [2]. Since then many papers devoted to the topological surface states (TSS) existing on the surfaces of such structures and which can be described by the pseudo-Dirac fermions [2–6] were published. The Dirac-like dispersion is observed due the uniaxial tensile strain along the (001) axis which lifts the degeneracy of the Γ\textsubscript{8} band by breaking the cubic symmetry at the Γ-point and opens the insulating gap. Against this gap the TSS are visible in a small energy area about 22 meV (for 3D HgTe TI) that makes such systems 3D TI [2].

The Dirac cone corresponds to a Dirac semimetal because there is no gap between the two cones, which would become hyperbolas when a gap is present. A normal insulator has a gap and a three-dimensional topological insulator is characterized by the bulk of the material having a gap while the surface has not. A Dirac semimetal, such as, for example, Na\textsubscript{3}Bi, is a three-dimensional system with a Dirac cone having a double degeneracy at the Fermi energy; Weyl semimetal has its valence and conduction bands touching each other at isolated points, around which the band structure forms non-degenerate three-dimensional Dirac cones. The apexes of the Dirac cones are called Weyl nodes.

In the case of the 2D systems based on CdTe/HgTe, the size of the HgTe QW makes the Dirac-like dispersion possible to be observed (for about 6.4 nm wide HgTe QW), which has been first predicted theoretically [7] and after that was proven by the experiment [8].

The Dirac cones are described by the four-component Dirac spinors satisfying the Dirac equation; when the mass is set equal to zero in the Dirac equation, it decouples into two equations known as the Weyl equations that have two component spinors as solutions.

In order to pass from Dirac semimetal to Weyl semimetal, the breaking of the time-reversal symmetry (TRS) or the breaking of the inversion symmetry is required. The breaking of TRS can be achieved in HgCdTe by magnetic impurities doping, namely in Hg\textsubscript{1−x−y}Cd\textsubscript{x}Mn\textsubscript{y}Te [9]. On the other hand, in order to achieve this effect in the superlattice based on the HgTe/CdTe multilayer structure, the broken inversion symmetry is required [10,11].

The breaking of inversion symmetry enforces each Dirac node to split into two pairs of separate Weyl nodes of same...
chirality at opposite momenta $+/−k_0$. This comes from the fact that if a Weyl node occurs at some momentum $k$, time-reversal symmetry requires that another Weyl node occurs at $−k$ with equal topological charge. This shows that the total topological charge associated with the entire Fermi surface must vanish. Hence, there must exist two more Weyl points of opposite topological charge at $k_0$ and $−k_0$.

In this paper the double-valley Dirac fermions in the strained 3D Hg$_{1−x}$Cd$_x$Te topological insulator with interface inversion asymmetry as well as for the asymmetric Hg$_{1−x}$Cd$_x$Te DQW are considered.

It was shown in the author’s previous work that symmetric structures with the same interfaces and the proper content of $x$-Cd in the Hg$_{1−x}$Cd$_x$Te compound together with the uniaxial tensile strain along the (001) direction and the proper width of the strained layers are enough to obtain the Dirac cone inside the gap between $Γ^{hh}_i$ and $Γ^{hh}_8$ [12]. In this paper it was also clearly shown that to obtain the interplay between two Dirac-like dispersions, such condition is extremely important and without that the double-valley Dirac semimetal (Weyl semimetal) cannot be realized. Here it is necessary to add some comments concerning terminology which is used here. In the literature devoted to the subject of the present discussion, the term Weyl semimetal is commonly accepted for describing the situation when the Dirac cone is split into two under the symmetry breaking. One should remember however, that Weyl equations are valid for massless particles; in the case when the Dirac cone is split into two under symmetry breaking, face inversion asymmetry as well as for the asymmetric Hg$_{1−x}$Cd$_x$Te DQW is studied.

The discussions carried out in most of the papers devoted to 3D HgCdTe TI [2,3] as well as to 2D HgTe TI [8] were focused on Dirac-like dispersion for 6.4 nm wide QW and the TSS for 3D TI against strained gap); 2) simple one/two-Dirac-cones model for QW/3D TI structures, respectively. These allow to explain the magneto-transport experiments [2,8,29,30].

In this work the eight-band $kp$ model [31,32] is used to calculate the dispersion relation for the two different types of HgCdTe-based TI: 1) the strained 3D TI 100 nm wide HgTe as well as the mixed HoCdTe layers with two different interfaces; 2) for DQW with the different $x$-Cd content in the QW and different widths of them.

This paper deals with the HgCdTe structures with broken inversion symmetry, but not the broken time-reversal symmetry as in other papers. All results presented here relate to 4.2K and were obtained by means of the methods elaborated in ref. [33]. The two structures which were considered fulfill the definition of topological insulator-normal insulator (TI-NI) multilayer structures [34].

For the case of 3D TI, two different interfaces correspond to IIA, while for the second, they correspond to asymmetric DQW structures, for which the chosen geometry corresponds to SIA. Such band engineering allows to get two linear dispersion cones in the nearest proximity of the $Γ$-point in the Brillouin zone.

Such linear dispersion together with band-touching points called Weyl nodes are very promising from the point of view of future applications. The charge carrier properties of such system are completely different in comparison with the known semiconductor structures used until now [35].

### 3D Hg$_{1−x}$Cd$_x$Te TI

As was mentioned above, so far many publications were devoted to the symmetric strained layers (about 75–80 nm wide HgTe) placed between two identical materials. The authors of these papers restricted their consideration only to different potentials originated from the different dielectric constants $ɛ$ on both surfaces of the structure in question, or to the external gate voltage (see, for instance, ref. [3]).

Without external voltage the different interfaces manifest themselves in the vicinity of $Γ_{hh}$ where the Dirac point is located at the $Γ$-point before hybridization [2].

The influence of the external voltage applied to 3D HgTe is observed only for TSS in the $k$-space far away from the $Γ$-point, when the Fermi level is located between the $Γ_6$- and $Γ_8$-states. In this case the external gate voltage is necessary for two reasons: first, to decrease the concentration, which is especially important for low carrier densities when
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Fig. 1: (Color online) $E(k)$ for (a) strained 100 nm wide Hg$_{0.865}$Cd$_{0.135}$Te and (b) strained 100 nm wide HgTe; obtained for non-symmetric cases structures — the sketches are visible in (c) and (d). The blue and the red solid curves represent the TSS for the interfaces between the CdTe and vacuum, respectively. The dotted colored curves show the lower part of the Dirac cones which is localized, in the case of (a), on the top of $\Gamma^h$ (red curve) and inside the strained gap (blue curve); and in the case of (b) on the top of $\Gamma^h$ (red curve) and deep inside the $\Gamma^h$ band (at $\approx -80$ meV).

...the broadening is stronger due to reduced screening [3]; and second, to split the TSS in order to observe two filling factors originating from two different independent 2DEG... A similar approach was used in case of pure 3D strained HgTe structures with the Nb as superconductor [36]. Here however, the low transparency the Nb-HgTe interfaces is responsible for the observed periodic oscillations of differential resistance.

First of all, the mixed Hg$_{1-x}$Cd$_x$Te strained 100 nm wide layers with the symmetric interfaces and $x$-Cd content equal 0.13 allows to get the Dirac point inside of the strained gap [12]. In this case we have two single no-crossing Dirac valleys at the $\Gamma$-point. In a similar structure, but with different materials at the two interfaces, the inversion symmetry breaking could manifest itself in more spectacular manner. The results of the numerical calculation of the energy dispersion for such case are shown in fig. 1 for: a) the strained mixed Hg$_{0.865}$Cd$_{0.135}$Te layers and b) strained 100 nm wide pure HgTe layers. In figs. 1(c) and (d) the sketches of the structures are shown for these two cases. The vacuum should be treated as a second different interfaces. It was defined by means of the boundary condition for the kp method [37].

For pure HgTe (fig. 1(b)) the different shapes of Dirac cones are clearly visible; they correspond to two different surfaces. The TSS belonging to the CdTe/HgTe interface are visible at the strained gap; they originate from the Dirac point which is deep inside the $\Gamma^h$-band, while the TSS at the HgTe/vacuum interface starts from the Dirac point which in this case is localized at the top of the $\Gamma^h$-band in the center of the Brillouin zone.

This situation becomes more complicated for the 100 nm wide strained Hg$_{0.865}$Cd$_{0.135}$Te layers — see fig. 1(a). The $x$-Cd content equal to $x = 0.135$ raises the Dirac point in energy scale. In addition, two different interfaces lead to the splitting of the Dirac cone into two (they are depicted as red and blue lines in fig. 1(a)). The apexes of the cones correspond to different energies in the $\Gamma$-point and it is important that the $E(k)$ curves are characterized by different slopes in the vicinity of the $\Gamma$-point.

This difference enforces different dispersion curves to intersect each other, so we can observe two Dirac valley nodes symmetrically arranged in the closed proximity of the $\Gamma$-point. It is worth mentioning that the TSS characterizing the interface at the vacuum side of the structure can be fitted by the Dirac-like Hamiltonian with the Fermi velocity two times greater than that for the pure 3D HgTe TI (see figs. 1(a) and (b)). This velocity can be calculated directly using the relation $\Delta E = h v_F \Delta k$ in the domain where dispersion is linear with respect to $k$. These results are shown in fig. 1 for both cases; the values written in red (fig. 1(a), (b)) mean the Fermi velocity for the interface on the vacuum side. The black curve (see inset in fig. 1(a)) corresponds to the linear dispersion for which the Fermi velocity is equal to $1.06 \times 10^6$ m/s.

Hg$_{1-x}$Cd$_x$Te DQW. – As was mentioned above, so far the DQW with the HgTe/HgCdTe materials were investigated for the structures with pure HgTe in QW and different widths. Just like in the previous case of the 3D TI, it will be interesting to explore the possibility to get two different Dirac cones in the case of a quantum 2D system.
Fig. 2: (Color online) The scheme of the DQW structures with the values of the $x$-Cd compounds and width of the QW as well as the barriers which were taken into account in the calculations (left panel). Right panel: $E(k)$ for DQW for three cases: (a) DQW#1, (b) DQW#2, (c) DQW#3 (obtained for the parameters summarized in the table in the left panel).

Based on the results presented in the author’s paper given in ref. [33], in the present paper the quantum 2D system, namely DQW were designed in order to search for the Dirac-like dispersion. This one occurs due to different $x$-Cd content in the Hg$_{1-x}$Cd$_x$Te compound and different widths of QW. The sketches of the DQW structures for which the calculation were done, are presented in fig. 2 (left part). The parameters of the CdTe/Hg$_{1-x}$Cd$_x$Te DQW structure, the widths of QW and the $x$-Cd content are summarized in the upper left panel in fig. 2. The calculations of the dispersion relations were carried out using these parameters as well as kp band parameters [29]; the results are presented in figs. 2(a)–(c). Using the obtained linear dispersion for the small values of the k-vector (ranging from 0 up to 0.1 nm$^{-1}$), we conclude that the Fermi velocity is equal to 0.95 × 10$^6$ m/s. This value is similar to that for graphene (1.06 × 10$^6$ m/s). To verify experimentally the existence of two double-valley Dirac cones in the case of the DQW structure should be easier, because of the simplicity of the experimental setup. Indeed, the contemporary technology for producing and preparing single QW based on Hg$_{1-x}$Cd$_x$Te should be sufficient to observe the corresponding effects in DQW structures.

Summary. – The aim of this work is to explore the consequences of the inversion symmetry breaking in the 3D and 2D mixed HgCdTe systems. As is shown, it is possible to obtain the double-valley Dirac cones in 3D TI as well as in DQW based on HgCdTe. The necessary conditions to get such shapes of the dispersion relations are: for the 3D TI one has a proper $x$-Cd content in the strained 3D HgCdTe layers together with the asymmetric interfaces; for HgCdTe DQW one has a proper value of the $x$-Cd content in each QW and a proper value of their width. So, the touching points of the valence and conduction bands with linear dispersion relation in their vicinities can be found in mixed 3D HgCdTe TI as well as in HgCdTe DQW systems. The effects related to the Dirac cones crossing in the structures examined in the paper could be experimentally verified in the cyclotron resonance and/or magneto-transport experiments.

Such band-touching points characterized by liner dispersion, called Weyl nodes, were for the first time predicted in ref. [38] and it looks like that they were already observed in strained Hg$_{1-x-y}$Cd$_x$Mn$_y$Te [9].

Experimental observation of our theoretical predictions, would be an important advancement in understanding the nature of correlated Dirac fermions in the unique state of matter, that is TI and Weyl semimetals. The consequences of Weyl dispersion was recently analyzed experimentally the existence of negative quadratic longitudinal magnetoresistance in similar structures. It seems, that the results of the present paper could be also interesting in regard to the rapid development of such exciting area of research as topological insulators and Weyl semimetals.

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