

About the paper “Two-dimensional massless electrons in an inverted contact”. B.A. Volkov and O.A. Pankratov, 1985.

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A discovery of topological insulators [1] and the booming interest in topologically protected electron states went to benefit for our paper of 1985 [2]. The effect that we thought was an interesting but exotic possibility occurred to be a precursor of a new quantum state of matter. Moreover, semiconducting compounds $Pb_{1-x}Sn_xTe$, the model systems that we considered, indeed turned out to be topological insulators [3].

The dynamics of the Bloch electrons in solids may drastically differ from that of the free Schrödinger particles. In particular, in narrow gap semiconductors there are two closely lying energy spectrum branches, the conduction and the valence band, which dominate their properties. This band structure is well described by the Dirac relativistic spectrum with the band gap ε_g playing the role of $2mc^2$. Henceforth these materials are described by the Dirac theory rather than the Schrödinger theory. Yet in contrast to the “true” Dirac particles, not only the value of the gap but also its sign (which determines the relative position of the two bands) matters here. The ordering of the bands is an observable with the band edges labeled by different symmetries of the wave functions. For example, in $PbTe$ the conduction band is odd and the valence band is even. This band ordering is, by convention, “normal” and it corresponds to $\varepsilon_g > 0$. On the contrary in $SnTe$ the bands are “inverted” i.e. the conduction band is even, the valence band is odd, and $\varepsilon_g < 0$.

The question that we asked to ourselves in 1985 was: what happens if we put together two materials with opposite signs of the band gap? Such an “inverted” contact can be fabricated e.g. by varying the composition in the alloy $Pb_{1-x}Sn_xTe$ between the normal ($PbTe$) and the inverted ($SnTe$) phases during the crystal growth. The answer comes from solving the Dirac equation with the variable band gap $\varepsilon_g(z)$. We found that, independently of a particular shape of the function $\varepsilon_g(z)$, this equation always has a solution localized at the interface, the only requirement being the change of a sign of $\varepsilon_g(z)$ on the boundary. In an (ideal) contact plane, the solution is, naturally, a plane wave. Herewith the energy depends linearly on the in-plane momentum – exactly as for the Dirac electrons in graphene [4]. However, in contrast to graphene, the spin structure of the wave functions is fixed i.e. the interface states show a giant spin splitting. As the spin degree of freedom is frozen, the interface particles obey the Weyl (not Dirac) equation. All these features are precisely the same as of the protected surface states on topological insulators [1]. Of course, the latter were not known at that time. In our paper, we only referred to a similarity with soliton states in the one-dimensional Peierls chains [5].

In the second part of the paper, we worked out the interface Landau levels in an external magnetic field applied perpendicular to the contact plane. A simple calculation gives a non-equidistant spectrum $(n) = \pm(\sqrt{2n\hbar v})/L$, where parameter v plays the same role as a speed of light in the Dirac Hamiltonian and L is a magnetic length. This formula was later repeatedly discussed in conjunction with an anomalous quantum Hall effect in graphene [4]. Having the Landau levels, we calculated the diamagnetic susceptibility and the quantum oscillations of the induced magnetic moment; we hoped that these signatures might be helpful for identifying the Weyl states in experiment.

To the best of my knowledge, the inverted $PbTe/SnTe$ contact has never been manufactured. Yet in 2007, the paper was published on a first experimental realization of a topological insulator – an “inverted” quantum well $CdTe/HgTe/CdTe$ [6]. Indeed, the $Cd_{1-x}Hg_xTe$ alloy also offers the band inversion and hence an opportunity for the Weyl states. In fact, we discussed this opportunity already in 1987 [7]. The situation here is somewhat more complicated because one of the bands is degenerate. It consists of the light and the heavy hole branches and only the light branch (which is mirrored to the conduction band) undergoes the inversion. As a result, the inverted state (occurring in $HgTe$) is metallic, or, more precisely, it is a semiconductor with zero band gap. This circumstance is harmful for the interface states. It is an advantage of the quantum well, that here the band degeneracy is lifted due to the quantization in z direction. This drives the system in an insulating state and enables the well-defined interface states.

Coming back to $Pb_{1-x}Sn_xTe$, it is nowadays clear that with these materials there is no need of fabricating the inverse contact to observe the Weyl particles. Namely, the “contact” to vacuum is enough! Since the “inverted” material $SnTe$ is, by itself, a topological insulator it always has the Weyl states on its surface. Their topological protection is guaranteed (in spite of an even number of the band extrema in the Brillouin zone) by the crystal symmetry [8].

In summary, a simple model that we considered almost 30 years ago, turned out to be a first example of a topological insulator. The origin of the topological nontriviality of the band structure in materials like $SnTe$ can be uncovered with a simple tight binding theory [9, 10] that B.A. Volkov and myself developed in the early 80-s for this material class. This work eventually guided us to ask a question: what happens if we bring two materials with opposite signs of the band gap in contact?

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