# Two-dimensional massless electrons in an inverted contact

B. A. Volkov and O. A. Pankratov
*P. N. Lebedev Physics Institute, Academy of Sciences of the USSR*

(Submitted 20 June 1985)
Pis'ma Zh. Eksp. Teor. Fiz. **42**, No. 4, 145–148 (25 August 1985)

A new type of semiconductor structures based on the contact of two materials with mutually inverted bands is proposed. A qualitative feature of this contact is the presence of electron states which have a two-dimensional linear spectrum and which do not depend on the transition region. The properties of an inverted contact in an external magnetic field are determined.

In the semiconductors $Pb_{1-x}Sn_x$ Te (or Se) the energy terms $L_6^{\pm}$ which form a band gap $\epsilon_g$ undergo an inversion as $x$ is increased (Fig. 1) (see Ref. 1, for example). The change in the work function is small in this case[2] and the diagram in Fig. 1 may be assumed symmetric with respect to the inversion point. An inhomogeneous structure which contains contacts between the semiconductors with a normal and inverted band arrangements can be synthesized by changing the composition during the growth of the crystal.[1)]

In a two-band approximation the energy spectrum of such a contact is described by a Dirac equation with a band gap which depends on the $z$ coordinate:

$$\begin{pmatrix} -\epsilon & i\epsilon_g/2+\sigma \mathbf{p} \\ -i\epsilon_g/2+\vec{\sigma}\mathbf{p} & -\epsilon \end{pmatrix} \begin{pmatrix} \chi_- \\ \chi_+ \end{pmatrix} = 0, \qquad (1)$$

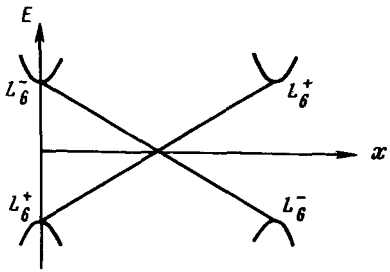


FIG. 1. Inversion of the $L_6^{\pm}$ bands in $Pb_{1-x}Sn_xTe(Se)$ involving a change in the composition.

 0021-3640/85/160178-04$01.00  

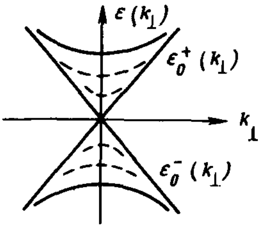

FIG. 2. Energy spectrum of the inverted contact. Solid curves—The Dirac (band) state and the Weyl state; dashed curves—additional branches which arise when the contact thickness is $l > l_0$.

where $\sigma$ are the Pauli matrices, $\mathbf{p} = -i\hbar(v_\perp\nabla_x, v_\perp\nabla_y, v_\parallel\nabla_z)$, the $z$ axis is directed along the trigonal axis of the crystal, and $\chi_\pm$ are the two-component spinors. If the signs of $\epsilon_g$ at the opposite sides of the contact are different, $[\epsilon_g(-\infty) < 0, \epsilon_g(+\infty) > 0]$, Eq. (1) will always have two solutions, which are localized at the contact, irrespective of the particular form of the function $\epsilon_g(z)$:

$$\Psi_\pm = A \begin{pmatrix} \pm\exp(-i\theta/2) \\ 0 \\ 0 \\ \exp(i\theta/2) \end{pmatrix} \exp\left\{-\frac{1}{2\hbar v_\parallel}\int_0^z \epsilon_g(z)dz + i\mathbf{k}_\perp\mathbf{r}\right\}, \tag{2}$$

where $\mathbf{k}_\perp = (k_x, k_y, 0)$ and $\exp(i\theta) = (k_x + ik_y)/k_\perp$. Substituting (2) into (1), we find that in the $(x, y)$ plane the functions $\psi_\pm$ satisfy the zero-mass Dirac equation which is equivalent to the Weyl equation in a unitary manner. We will therefore call the corresponding nondegenerate massless spectrum

$$\epsilon_0^\pm(\mathbf{k}_\perp) = \pm\hbar v_\perp k_\perp \tag{3}$$

the Weyl spectrum (Fig. 2). A two-dimensional nondegenerate spectrum also occurs in a normal heterogeneous transition due to the spin-orbit interaction which arises as a result of the inhomogeneity of the system,[3] but the spin splitting of the bands is small in this case.

To find the total spectrum of the contact, we must express $\chi_-$ in terms of $\chi_+$ with the help of Eq. (1) and then substitute the result into Eq. (2). We then find

$$(\mathbf{p}^2 + U(z, \sigma_z) - \epsilon^2)\chi_+ = 0, \tag{4}$$

where

$$U(z, \sigma_z) = (\epsilon_g^2 + 2\hbar v_\parallel \sigma_z \partial\epsilon_g/\partial z)/4. \tag{5}$$

In its origin, spectrum (3) at $k_\perp = 0$ is approximately equal to the soliton spectrum in a one-dimensional Peierls insulator,[4] so that $\epsilon_g(z)$ can be chosen in the form

$$\epsilon_g(z) = \epsilon_g(\infty)\tanh(z/l). \tag{6}$$

Here

$$U(z, \sigma_z) = (\epsilon_g^2(\infty)/4)[1 - (1 - \sigma_z l_0/l)\cosh^{-2}(z/l)], \tag{7}$$

where $l_0 = 2\hbar v_\parallel/\epsilon_g(\infty)$, and Eq. (4) can be solved analytically.[5] In addition to the Dirac spectrum, this equation has, at $\epsilon^2 > \epsilon_g^2(\infty)/4$, several solutions, which are localized at the contact, with the energies

$$\epsilon^{\pm}_{n\sigma}(\mathbf{k}_{\perp}) = \pm\ \{[1-(1-(n+(1+\sigma)/2)l_0/l)^2]\,\epsilon_g^2(\infty)/4+\ \hbar^2 v_{\perp}^2 \mathbf{k}_{\perp}^2\}^{1/2}\,, \qquad (8)$$

where $n$ are integers, and $0 \leqslant n+(1+\sigma)/2 \leqslant l/l_0$. At $l/l_0 > 1$, in addition to the Weyl branch ($n=0$, $\sigma=-1$), we see doubly degenerate branches ($n,\sigma=1$; $n+1$; $\sigma=-1$). At $l \gg l_0$ these branches form a quasi-continuous spectrum. If $l/l_0$ is an integer, potential (7) is a nonreflecting potential[5] (the wave functions of a three-dimensional Dirac spectrum do not contain a reflected wave in the asymptotic limit $z \to \pm\infty$).

The electron density in the inverted contact with $l=l_0$ and chemical potential $\mu=0$ is constant and there is no internal electric field. There is also no spin density perturbation. The field produced at $\mu \neq 0$ is small[2] because of the large ($10^3$) dielectric constant of $A^4B^6$.

The Landau-level spectrum of the Weyl branch in a magnetic field $\mathbf{H}$ parallel to the $z$ axis can be found through the replacement $\mathbf{p} \to \mathbf{p}(ev_{\perp}/c)\mathbf{A}$:

$$\epsilon^{\pm}(n) = \pm\sqrt{2n}\,\hbar v_{\perp}/L\,,\quad n = 0, 1, 2, \dots\,, \qquad (9)$$

where $L^2 = c\hbar/eH$. Since $\sqrt{2}\hbar v_{\perp}/L = [\epsilon_g(\infty)\hbar\omega_c]^{1/2} \gg \hbar\omega_c$ [$\omega_c$ is the cyclotron frequency of the Dirac electrons with a mass $m_c = \epsilon_g(\infty)/2v_{\perp}^2$], the splitting of the Weyl states is much greater than that of the Dirac states. Summing over the levels (9) makes it possible to find the $\Omega$ potential and the susceptibility

$$\chi = -\frac{1}{Sl_0}\frac{\partial^2\Omega}{\partial H^2} = -\frac{e^2 v_{\perp}^2}{48\pi\hbar v_{\parallel} c^2}\,\frac{\epsilon_g(\infty)}{T\cosh^2(\mu/2T)} \qquad (10)$$

per unit volume of the contact in a weak field $\hbar v_{\perp} \ll LT$. At $T_{\max} = |\mu|/2\sqrt{3/5}$ the susceptibility reaches a maximum value Fig. (3):

$$\chi_{\max} = -\frac{e^2 v_{\perp}^2}{96\pi\hbar v_{\parallel} c^2}\,\frac{\epsilon_g(\infty)}{|\mu|}\,. \qquad (11)$$

The first factor in (11) is on the order of the diamagnetic Landau susceptibility $\chi_L$. For a semiconductor which is approximately the same as an intrinsic semiconductor we have $\epsilon_g(\infty)/|\mu| \gg 1$ and $\chi_{\max} \gg \chi_L$. As for the diamagnetism of the Dirac electrons, it is intensified in comparison with $\chi_L$ only by the logarithmic factors[6] $\ln|m_c v_{\parallel}^2/\epsilon_g(\infty)|$.

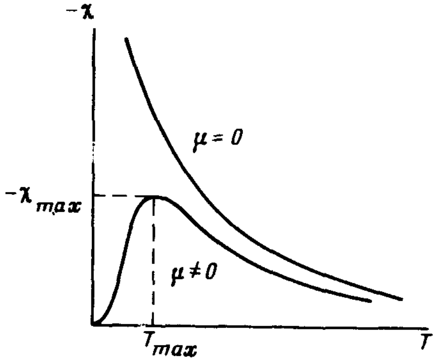


FIG. 3. Temperature dependence of the magnetic susceptibility of the Weyl electrons in a weak field. The chemical potential $\mu = 0$ corresponds to a half-filled Weyl spectrum.

In a strong field $\hbar v_\perp \gg LT$, the contribution to $\Omega$, which oscillates with respect to $1/H$, causes the magnetic-moment oscillations

$$M/S = -\frac{1}{S}\frac{\partial\Omega}{\partial H} = \frac{|\mu| e}{4\pi\hbar c}\sum_{m=0}^{\infty} x\,\theta(m+1-x)\theta(x-m), \tag{12}$$

where $\theta(x)$ is the theta function, $x = 2\pi L^2 n_S$, and $n_S = \mu^2/4\pi\hbar^2 v_\perp^2$ is the excess density of the Weyl electrons (holes) per unit area. The function (12) has a sawtooth shape as in the case of 2D electrons with a quadratic dispersion law.[7] The oscillation period of the momentum of the Weyl electrons with respect to the reciprocal of the field is $e/2\pi\hbar c n_S$. The ratio of this period to the oscillation period of the Dirac electrons is $[\mu^2 - \epsilon_g^2(\infty)/4]/\mu^2 \ll 1$.

The oscillation phenomena involving the Weyl electrons should be seen in the classical and ultraquantum fields in the case of the Dirac electrons.

Numerical estimates of the parameters of the inverse contact for $Pb_{0.72}Sn_{0.18}Te$ [$\epsilon_g(\infty) = 90$ meV, $v_\parallel = 2.24\times 10^7$ cm/s, $v_\perp = 8\times 10^7$ cm/s] show that its characteristic thickness is $l_0 = 33$ Å and its density is $n_S \sim 10^{11}$ cm$^{-2}$ for $\mu \sim \epsilon_g(\infty)/2$. In a field $H = 10^4$ G the level $\epsilon^+(1) = 30$ meV, and the entire band gap is spanned by five Landau levels. Here the volume concentration in a single level is $n_H = (2\pi L^2 l_0)^{-1} \sim 10^{17}$ cm$^{-3}$. The density of the Dirac electrons can therefore be controlled with the help of the magnetic field in a superlattice consisting of inverted contacts. In a superlattice of this sort contributions (10) and (12) of the Weyl electrons to the magnetic response are not masked by the volume.

The Weyl states can arise naturally due to the fluctuations of the composition in alloys such as PbSnTe or CdHgTe and at the twinning boundaries in semimetals of the V group. Since the spectrum of these states spans the entire band gap, defects of this sort are the effective centers of the radiationless recombination which can be suppressed by a strong magnetic field.

[1)] Such a contact can also be established with $Cd_xHg_{1-x}Te$, where the electron and light-hole bands are inverted. Here, however, there is also a heavy-hole band which masks the specific features of the inverted contact.


[1] G. Nimtz, B. Schlicht, and R. Dornhaus, Narrow-Gap Semiconductors, Springer Tracts in Modern Physics, 1983, p. 98.
[2] M. Kriechbaum, K. E. Ambrosch, E. J. Fanter, H. Clemens, and G. Bauer, Phys. Rev. B **30**, 3394 (1984).
[3] Yu. A. Bychkov and É. I. Rashba, Pis'ma Zh. Eksp. Teor. Fiz. **39**, 66 (1984) [JETP Lett. **39**, 78 (1984)].
[4] S. A. Brazovskiĭ, Zh. Eksp. Teor. Fiz. **78**, 677 (1980) [Sov. Phys. JETP **51**, 342 (1980)].
[5] L. D. Landau and E. M. Lifshitz, Kvantovaya mekhanika (Quantum Mechanics), Fizmatgiz, Moscow, 1963, pp. 97 and 105 [Pergamon Press, Oxford, 1965].
[6] L. A. Fal'kovskiĭ, Zh. Eksp. Teor. Fiz. **80**, 334 (1981) [Sov. Phys. JETP **53**, 170 (1981)].
[7] R. Peierls, Zs. f. Physik **81**, 186 (1933).


Translated by S. J. Amoretty