Types of nonuniform structures, boundary electron states, and chiral anomaly in semiconductors with Dirac bands

O. A. Pankratov

P. N. Lebedev Physics Institute, Academy of Sciences of the USSR, Moscow

(Submitted 19 November 1986)

Pis'ma Zh. Eksp. Teor. Fiz. **45**, No. 2, 82–85 (25 January 1987)

All types of nonuniform semiconductor structures are classified on the basis of an effective Dirac Hamiltonian. For one version—an antiferromagnetic domain wall—there is an analogy with the chiral anomaly, manifested as the presence of a magnetic moment perpendicular to the plane of the wall.

The classification of semiconductor heterojunctions which is presently being used is based on a comparison of the width of the energy gap ϵ_g and the work function φ of the materials in contact.[1] However, $\epsilon_g(\mathbf{r})$ and $\varphi(\mathbf{r})$ do not exhaust the list of physical fields which might be responsible for a nonuniformity.

For a two-band semiconductor, whose energy spectrum can be described by the

Dirac equation (e.g., IV–VI compounds[2]), the Hamiltonian in the effective-mass approximation is actually completely spherically symmetric (if the mass anisotropy is ignored). This symmetry allows perturbations corresponding (in relativistic notation) to the covariant bilinear forms

$$[-m_0 + v\gamma^\mu (i\partial_\mu - eA_\mu) + \gamma_5 P + i\gamma^\mu \gamma_5 M_\mu + \frac{i}{2}\gamma^\mu \gamma^\nu F_{\mu\nu}]\psi = 0, \tag{1}$$

where $m_0(\mathbf{r}) \equiv \epsilon_g(\mathbf{r})/2$, $A_\mu = (\varphi, -\mathbf{A})$, $P(\mathbf{r})$ is a pseudoscalar, $M_\mu(\mathbf{r}) = (M_0, \mathbf{M})$ is a pseudovector, and $F_{\mu\nu}(\mathbf{r}) \equiv (\mathbf{E}, \mathbf{B})$ is an antisymmetric tensor ($\mathbf{E}$ and $\mathbf{B}$ are polar and axial vector fields which are by no means necessarily electric and magnetic fields). Instead of the velocity of light in (1) we have the interband velocity matrix element v, which may be regarded as a scalar if we ignore the crystallographic anisotropy. In the steady state, the Hamilton's form of Eq. (1) is

$$\begin{pmatrix} e\varphi + m_0 + (\mathbf{M}+\mathbf{B})\vec{\sigma} - \epsilon & v\vec{\sigma}(\hat{\mathbf{p}} - e\mathbf{A}) - i\vec{\sigma}\mathbf{E} + iP - M_0 \\ \text{H.a.} & e\varphi - m_0 + (\mathbf{M}-\mathbf{B})\vec{\sigma} - \epsilon \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0. \tag{2}$$

Since we are actually dealing with only the spatial symmetry, not the complete Lorentz group, the quantities $\mathbf{M}$ and M_0 are independent, as are $\mathbf{B}$ and $\mathbf{E}$, and as are φ and $\mathbf{A}$.

At an ordinary heterojunction φ and m_0 would be functions of the coordinate z. A change in the sign of $m_0(z)$ corresponds to an inverse contact.[3,4] A perturbation of $\mathbf{E}$ occurs in ferroelectric semiconductors. A nonuniformity of $\mathbf{E}(z)$ may take the form of, for example, a domain wall.[5] As was shown in Refs. 3–5, two-dimensional boundary electron states exist in nonuniform structures of this sort.[1)]

The diagonal terms of $(\mathbf{M} \pm \mathbf{B})\vec{\sigma}$ may be thought of as the contribution of remote bands to the electron and hole g-factors.[2] If we return to the explicit form of the basis functions,[6] we easily see that the matrix element iP corresponds to an interaction with an antiferromagnetic subsystem, while M_0 corresponds to a spin-orbit perturbation due to an odd component of the crystal potential.

For a uniform antiferromagnetic semiconductor, omitting from (2) all external fields except $P(z) = P$, we find

$$\epsilon(k_z, \mathbf{k}_\perp) = \pm [m_0^2 + P^2 + \hbar^2 v^2 (k_z^2 + k_\perp^2)]^{1/2}, \tag{3}$$

where k_z and $\mathbf{k}_\perp$ are the projections of the quasimomentum onto the z axis and onto the perpendicular plane. In the presence of a domain wall we would have $P(z \to \pm\infty) = \pm P$ and $P > 0$; squaring (2), we find the wave equation of supersymmetric quantum mechanic[2)]

$$[(v\sigma_z \hat{p}_z \mp iP(z))(v\sigma_z \hat{p}_z \pm iP(z)) + \hbar^2 v^2 k_\perp^2 + m_0^2 - \epsilon^2]\psi_{\substack{2\\1}} = 0. \tag{4}$$

The zero mode of this equation, $(\psi_1^{(0)}, \psi_2^{(0)})$ corresponds to 2D states which are localized near the domain wall and whose spectrum

$$\epsilon_0(\mathbf{k}_\perp) = \pm (m_0^2 + \hbar^2 v^2 k_\perp^2)^{1/2} \tag{5}$$

is not degenerate because of the fixed spin structure of the functions $\psi_2^{(0)} \sim |\downarrow\rangle$ and $\psi_1^{(0)} \sim |\uparrow\rangle$[3]

In a magnetic field H directed parallel to the z axis, Eq. (2) becomes

$$\begin{pmatrix} m_0 - \epsilon & (v\sigma_z \hat{p}_z + iP(z)) + \sigma_+\pi_- + \sigma_-\pi_+ \\ \text{H.a.} & -m_0 - \epsilon \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0, \tag{6}$$

$\sigma_\pm$ and $\pi_\pm$ are "raising" and "lowering" spin and orbital operators, and we have the commutation relation $[\pi_+, \pi_-] = -2|e|\hbar H/c$. Since for the states of the zero mode we have $\sigma_+\psi_1^{(0)} = \sigma_-\psi_2^{(0)} = 0$ and $[v\sigma_z\hat{p}_z \pm iP(z)]\psi_{\substack{2\\1}}^{(0)}(z) = 0$, we find from (6) the Landau levels

$$\epsilon_0(n) = \pm(m_0^2 + 2n\hbar^2 v^2/L^2)^{1/2}; \quad n = 1, 2, 3, \ldots$$
$$\epsilon_0(0) = -m_0 \operatorname{sign} H, \tag{7}$$

where $L = (c\hbar/|eH|)^{1/2}$ is a magnetic length. At $H > 0$, the level $+m_0$ is absent, since we have $\pi_+\varphi_2^{(0)} \neq 0$, while the normalized solution of the equation $\pi_-\varphi_1^{(0)} = 0$, which corresponds to the level $-m_0$, exists. If the sign of H is changed, the operators π_+ and π_- exchange roles, with the result that the level $-m_0$ disappears, and a state $\epsilon_0(0) = +m_0$ appears. The symmetry of the spectrum under the replacement $\epsilon \to -\epsilon$ is thus broken.

A "hop" of the Landau zero level and thus a jump in the energy upon the inversion of the field imply the presence of a magnetic moment which is oriented along the z axis. As a result, as in (2 + 1) electrodynamics,[8] we loose the symmetry under reflection through a plane passing through this axis, despite the fact that in the limit $H \to 0$ the symmetry $\epsilon \to -\epsilon$ is restored.

In electrodynamics, a chiral anomaly is manifested through a vacuum charge density and a vacuum current density, both universal (in the given field). Since in any heterostructure the chemical potential μ is fixed by the volume and is in principle arbitrary, in our case these quantities are not universal, being determined by the filling of the zero mode. On the other hand, the magnetic moment per unit area,

$$\mathcal{M} = -\frac{1}{2H}[\Omega(H) - \Omega(-H)] = \frac{T}{2\phi_0}(\operatorname{sign} P)\ln\frac{1 + \exp[(\mu + m_0)/T]}{1 + \exp[(\mu - m_0)/T]} \tag{8}$$

is, at $T = 0$ and $\mu > m_0$, equal to simply (m_0/ϕ_0) sign P and does not depend on $|P|$! (See Fig. 1; here $\phi_0 = 2\pi\hbar c/|e|$ is the quantum of flux.) In the limit $P \to 0$, the localization length of the moment along the z axis increases without bound, so that the volume density of the moment tends towards zero. The moment $\mathcal{M}$ arises from the presence of a special direction, specified by grad $P(z)$ in the third dimension [which is of course not present in (2 + 1) electrodynamics].

We conclude with a brief discussion of the field $M_0(\mathbf{r})$. Retaining only the perturbation $M_0(\mathbf{r})$ in (2), we find

$$v\vec{\sigma}\hat{\mathbf{p}}\psi_1 = [-M_0(\mathbf{r}) \pm \sqrt{\epsilon^2 - m_0^2}]\psi_1, \tag{9}$$

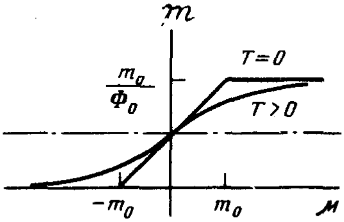

FIG. 1. Density of the magnetic moment of an antiferromagnetic domain wall versus the chemical potential μ at various temperatures. The interval $-m_0<\mu<m_0$ corresponds to the energy gap, and ϕ_0 is the quantum of flux.

where $|\epsilon|>m_0$. In contrast with the other fields which we have considered, the nonuniformity $M_0(r)$ apparently cannot localize electrons. This fact is obvious for a 1D structure $M_0(z)$, since

$$\psi_1^{(\pm)}(z) \sim \exp\left\{ \frac{i}{\hbar v} \int_0^z [-M_0(z) \pm \sqrt{\epsilon^2 - m_0^2}]dz \right\} \tag{10}$$

We accordingly restrict the discussion to the case $M_0(r) \equiv M_0 = \text{const}$. If there is no external magnetic field, the energy spectrum becomes

$$\epsilon(\mathbf{k}) = \pm [m_0^2 + (M_0 \pm \hbar v |\mathbf{k}|)^2]^{1/2} \tag{11}$$

In a magnetic field $H\|z$, the Landau zero subbands loose their symmetry under the replacement $k_z \to -k_z$:

$$\epsilon_\pm(n, k_z) = \pm \{m_0^2 + (M_0 \pm \hbar v \sqrt{k_z^2 + 2n/L^2})^2\}^{1/2}; \quad n = 1, 2, 3, \dots \tag{12}$$
$$\epsilon(0, k_z) = \pm \{m_0^2 + (M_0 - \hbar v k_z)^2\}^{1/2}$$

The extrema of the zero subbands shift an amount $k_0 = M_0/\hbar v$ in the direction of the magnetic field. For a massless two-component Weyl equation in $(3+1)$ dimensions, the asymmetric zero mode created by the magnetic field intersects the axis $\epsilon = 0$, giving rise to an Adler-Bell-Jackiw current anomaly.[9] In our case, the equation is a four-component equation, so that a current state does not arise. An energy spectrum of the type in (11), (12) may arise by virtue of the spin-orbit interaction in a semiconductor lacking a center of symmetry. In particular, the conduction band of tellurium is of this nature.[10]

I wish to thank S. M. Apenko for calling my attention to Ref. 9.

[1)]The term $i\hat{\sigma}\mathbf{E}$ corresponds to the anomalous magnetic moment of a Dirac particle. For a neutron in the electric field of a charged plate, there thus exist supersymmetric bound states, according to Ref. 5, with an energy which depends on the two-dimensional momentum.
[2)]This case is mathematically equivalent to an inverse contact in a uniform antiferromagnet[7] [$P(z) = \text{const}$; $m_0 = m_0(z)$], since the corresponding Hamiltonians are coupled by a unitary transformation.

[1]A. P. Silin, Usp. Fiz. Nauk **147**, 485 (1985) [Sov. Phys. Usp. **28**, 972 (1985)].
[2]G. Nimtz, B. Schlicht, and R. Dornhaus, Narrow-Gap Semiconductors, Springer Tracts in Modern Physics, Vol. 98, 1983.

[3]B. A. Volkov and O. A. Pankratov, Pis'ma Zh. Eksp. Teor. Fiz. **42**, 145 (1985) [JETP Lett. **42**, 178 (1985)].
[4]O. A. Pankratov, S. V. Pakhomov, and B. A. Volkov, Solid State Commun. No. 8 (1986).
[5]B. A. Volkov and O. A. Pankratov, Pis'ma Zh. Eksp. Teor. Fiz. **43**, 99 (1986) [JETP Lett. **43**, 130 (1986)].
[6]B. A. Volkov, O. A. Pankratov, O. A. Sazonov, Zh. Eksp. Teor. Fiz. **85**, 1395 (1983) [Sov. Phys. JETP **58**, 809 (1983)].
[7]F. V. Kusmartsev and A. M. Tsvelik, Pis'ma Zh. Eksp. Teor. Fiz. **42**, 207 (1985) [JETP Lett. **42**, 257 (1985)].
[8]G. W. Semenoff, Phys. Rev. Lett. **53**, 2449 (1984).
[9]H. B. Nielsen and M. Ninomiya, Phys. Lett. **130b**, 389 (1983).
[10]J. Blinowski, G. Rebmann, C. Rigaux, and J. Mycielski, J. Phys. (Paris) **38**, 1139 (1977).

Translated by Dave Parsons