Physical Realization of the Parity Anomaly in Condensed Matter Physics

Eduardo Fradkin and Elbio Dagotto
Department of Physics, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801

and

Daniel Boyanovsky
Stanford Linear Accelerator Center, Stanford, California 94305
(Received 30 June 1986)

We show that a PbTe-type narrow-gap semiconductor with an antiphase boundary (or domain wall) has currents of abnormal parity and induced fractional charges. A model is introduced which reduces the problem to the physics of a Dirac equation with a soliton in background electric and magnetic fields. We show that this system is a physical realization of the parity anomaly.

PACS numbers: 71.50.+t, 05.30.Fk, 11.30.Er, 11.30.Rd

In the past few years topological and macroscopic quantum effects have attracted considerable attention in condensed matter physics. Perhaps the most famous case is the quantum Hall effect, in both its integral and fractional forms.[1] At the same time the phenomenon of the parity anomaly in $(2+1)$-dimensional quantum electrodynamics $(\mathrm{QED})_{2+1}$ was discovered within the framework of field theory.[2] Several attempts have been made to find analogs of the parity anomaly in condensed matter systems. It was first proposed that the integral quantum Hall effect may be related to the parity anomaly[3,4] in $(\mathrm{QED})_{2+1}$. It was later shown that, on the basis of symmetry, they are quite different phenomena.[5,6] Semenoff[7] recently proposed the study of "two-dimensional graphite" as a way to exhibit effects of the parity anomaly. He showed that the abnormal-parity current of $(\mathrm{QED})_{2+1}$ is canceled as a result of the pervasive fermion-doubling problem.[8] Since interlayer couplings in actual graphite destroy the analog relativistic behavior of the electrons, his analysis may only hold for a system with just one layer.

In this paper we point out the existence of a lattice system in three dimensions which does exhibit the parity anomaly of QED in two dimensions. We consider a narrow-gap semiconductor of the PbTe type.[9] These systems have a rocksalt structure with the gap between the conduction and valence bands closest at the L points of the Brillouin zone. This feature is the consequence of the strong spin-orbit interaction. Next we consider the effects of an antiphase boundary (or domain wall) on the electronic states. For simplicity consider a wall on the (001) axis. We show that in the presence of the wall a number of surface states appear ("zero modes"). For a *uniform magnetic field perpendicular to the wall,* a net charge is accumulated *on the wall.* If *a uniform electric field parallel to the wall* is applied a current of abnormal parity is shown to exist. These currents are *independent* of the sign of the magnetic field and should be observable in a Hall-type experiment as currents that do not change sign when $\mathbf{B}\to-\mathbf{B}$.

From a formal point of view our analysis relies on the fact that the states close to the Fermi energy of a narrow-gap semiconductor with an antiphase boundary are equivalent to a system of four species of massive relativistic fermions in the background of a scalar soliton in $3+1$ dimensions. Our analysis is then complementary to the seminal work of Callan and Harvey[10] who considered a (2+1)-dimensional theory with a scalar soliton and a (3+1)-dimensional theory with a string. In both cases there is an axial anomaly in the Hilbert space of the states on the defect. In a recent paper Volkov and Pankratov[10] proposed a similar analogy for a PbTe-SnTe heterojunction.[11] There are also amusing analogies between this problem and the quasiparticle currents in the A phase of ^{3}He with a texture.[12]

Consider first a phenomenological tight-binding model which describes the electronic states that nearly cross at the L points. Let us consider first a system without a wall. The Pb atoms then sit at one sublattice of the rocksalt "cubic" structure and the Te atoms at the surrounding sites. If we neglect the effects of the other bands we can write a simple tight-binding model with two orbitals per site (spins up and down) with a spin-dependent hopping term which represents the spin-orbit interaction. We write

$$H=\sum_{\substack{\mathbf{r},\mu=1,2,3\\ \alpha,\beta=\uparrow,\downarrow}} T\phi_\alpha^\dagger(\mathbf{r})\sigma_\mu^{\alpha\beta}\phi_\beta(\mathbf{r}+\hat{\mathbf{e}}_\mu)+\text{H.c.}+\sum_{\mathbf{r},\alpha=\uparrow,\downarrow} M(-1)^{x+y+z}\phi_\alpha^\dagger(\mathbf{r})\phi_\alpha(\mathbf{r}), \tag{1}$$

where $\phi_\alpha(\mathbf{r})$ destroys an electron of spin α at $\mathbf{r}$, $\{\hat{\mathbf{e}}_\mu\}$ are nearest-neighbor lattice vectors, and $\{\sigma_\mu\}$ are the three Pauli matrices. We have assumed that one type of atoms sit at the sublattice $x+y+z=$even, with site energy $+M$ and that the other type sit at the sublattice $x+y+z=$odd, with site energy $-M$. T is a hopping amplitude. It is easy to show that the single-particle spectrum of this system is

$$E(\mathbf{k}) = \pm \left[M^2 + T^2 \sum_{\mu=1}^{3} \cos^2 k_\mu \right]^{1/2}. \tag{2}$$

The gap is smallest at the L points of the Brioullin zone, $(\pm\pi/2, \pm\pi/2, \pm\pi/2)$, and equals $2M$.

It is easy to introduce a domain wall into this system. We want to exchange Pb atoms with Te atoms, say, to the right of the wall. This is accomplished by our writing a z-dependent site term $M(z)$ with the property $\lim_{z\to\pm\infty} M(z) = \pm M$. For a sharp wall $M(z)$ is a step function. After spin diagonalization, and for appropriate choice of phases, we can show that the Hamiltonian of Eq. (1) is the same as the Hamiltonian of two decoupled Kogut-Susskind fermions, a particular way of discretizing the Dirac equation.[13] Thus we write

$$\phi_\alpha(\mathbf{r}) = i^{x+z}(-1)^{y(y+1)/2}(\sigma_1^x \sigma_2^y \sigma_3^z)_{\alpha\beta}\psi_\beta(\mathbf{r}), \tag{3}$$

and the Hamiltonian now is

$$H = \sum_{\mathbf{r},\alpha} T\{\psi_\alpha^\dagger(\mathbf{r}) i[\psi_\alpha(\mathbf{r}+\hat{\mathbf{e}}_1) - \psi_\alpha(\mathbf{r}-\hat{\mathbf{e}}_1)] - \psi_\alpha^\dagger(\mathbf{r})(-1)^{x+y}[\psi_\alpha(\mathbf{r}+\hat{\mathbf{e}}_2) + \psi_\alpha(\mathbf{r}-\hat{\mathbf{e}}_2)]$$
$$+ \psi_\alpha^\dagger(\mathbf{r}) i(-1)^{x+y}[\psi_\alpha(\mathbf{r}+\hat{\mathbf{e}}_3) - \psi_\alpha(\mathbf{r}-\hat{\mathbf{e}}_3)]\} + \sum_{\mathbf{r},\alpha} M(z)(-1)^{x+y+z}\psi_\alpha^\dagger(\mathbf{r})\psi_\alpha(\mathbf{r}). \tag{4}$$

From the results of Ref. 13 it is easy to show that, for states near the Fermi energy, it is possible to write Eq. (4) in the standard continuum form with two species (four including spin) of Dirac fermions,

$$\tilde{H} = \sum_{a=\uparrow,\downarrow} \int d^3x \{\eta_a^\dagger i\boldsymbol{\alpha}\cdot\nabla\eta_a + \chi_a^\dagger i\boldsymbol{\alpha}\cdot\nabla\chi_a + m(z)\eta_a^\dagger\beta\eta_a + m(z)\chi_a^\dagger\beta\chi_a\}, \tag{5}$$

where $\boldsymbol{\alpha},\beta$ are the Dirac matrices, η and χ are the two species of fermions, and $m(z) = M(z)/T$. The eight fields needed to make up two Dirac fermions are linear combinations of amplitudes on the sites of a cube.[13] What is crucial for our results is that *the mass term $m(z)$ has the same sign for all species* (and spin orientations). While this is possible for fermions in three dimensions, this is not the case in two dimensions. Two-dimensional lattice fermions have a continuum limit with two species of two-component Dirac fermions with opposite masses and hence opposite parity.[7] This is a consequence of the inversion symmetry of any Bravais lattice in two space dimensions.[14]

Let us consider the states in the system described by Eq. (5) first without an electromagnetic field. Since all four species couple to the soliton in the same way we need to consider a problem with just one species and assume a fourfold degeneracy of the states. We will comment below on the effects of various degeneracy-lifting perturbations.

(i) *Zero electromagnetic field.*—It is easy to solve for the states in a background of a soliton. Let $\eta_a(\mathbf{x})$ be a four-component spin. The Dirac equation in the background of a soliton along the z direction is

$$[i\boldsymbol{\partial} - m(z)]\eta(\mathbf{x}) = 0, \tag{6}$$

with use of the standard Bjorken-Drell notation.[15] The symmetry of this Hamiltonian suggests that we look for factorized solutions of the form

$$\eta_a(\mathbf{x}) = \phi_a(\mathbf{x}_\perp) f(z), \tag{7}$$

where $\phi_a(\mathbf{x}_\perp)$ is a four-spin and a function of the x,y coordinates and $f(z)$ is a scalar function of z. We now look for solutions which are normalizable (i.e., square integrable) in the z direction. This last requirement implies that

$$\gamma_3\phi(\mathbf{x}_\perp) = -i\phi(\mathbf{x}_\perp) \tag{8}$$

for $m(z)|_{z\to+\infty} \to +m > 0$, and

$$[-\partial_z - m(z)]f(z) = 0, \tag{9}$$

the solution of which is

$$f(z) = f(0)\exp\left[-\int_0^\infty dz' m(z')\right]. \tag{10}$$

The requirement that η be a solution of Eq. (6) forces

$$i\boldsymbol{\partial}_\perp\phi(\mathbf{x}_\perp) = 0 \tag{11}$$

to be satisfied (with use of an obvious notation). Equation (11) says that the modes bound to the wall are massless and the constraint equation (8) means that there are only two components. This is precisely a massless Dirac-Weyl fermion in 2+1 space-time dimensions. The other states can be found with similar arguments. There are continuum bulk states [i.e., delocalized with a gap of the order of $m(\infty)$] and possibly other massive bound states depending on the precise profile of the wall. For a sharp wall only the "zero modes" found above survive. These zero modes are closely related to the zero modes or midgap states of one-dimensional theories[16] with solitons and in systems such as polyacetylene. Following the one-dimensional analogy it is natural to ask if the filled Fermi sea of our problem has fractional charge. General arguments, valid in the one-dimensional case, as well as in our case, indicate that the charge Q induced by the wall is the spectral asymmetry[17,18]

$$Q = -\tfrac{1}{2}e\int_0^\infty [\rho_W(E) - \rho_W(-E)]dE, \tag{12}$$

where $\rho_W(E)$ is the density of states at energy E in the presence of a wall. The fact that Eq. (5) has particle-hole symmetry and that the zero modes have a vanishing density of states implies that $Q = 0$ in the absence of external electromagnetic fields.

(ii) *Nonzero electromagnetic fields.*—The presence of external static magnetic and/or electric fields drastically alters the situation. Consider first the case of a constant uniform magnetic field of strength B *pointing in the z direction.* Equation (6) now is

$$[i\boldsymbol{\partial} - (e/c)A - m(z)]\eta(\mathbf{x}) = 0, \tag{13}$$

where the vector potential A_μ equals $(0,0,Bx,0)$ in the Landau gauge. The point here is that the solutions of Eq. (13) (i.e., the relativistic Landau levels) appear in pairs of energies $\pm E$ (particle-hole symmetry) but there is a set of unpaired zero-energy modes, i.e., Landau levels with zero energy. Their wave functions are

$$\eta_0(\mathbf{x}) = \begin{pmatrix}1\\0\\0\\0\end{pmatrix} \exp\left[-\int_0^z dz' \frac{1}{\hbar} m(z')\right] \exp\left[\frac{iyk_y}{\hbar} - \frac{eB}{2\hbar c}(x-x_0)^2\right], \tag{14}$$

with degeneracy $4(BA/2\pi)e/\hbar c$ (where A is the area of the wall), when we take into account the fourfold degeneracy. The spectrum is still symmetric around $E = 0$. Thus Eqs. (12) and (14) imply that the induced charge is $Q = (e/2)N_0$, where N_0 is the number of zero modes. Using the degeneracy of the lowest Landau level we get

$$Q/A = -(B/4\pi)(e^2/\hbar c)\times 4 \tag{15}$$

for the charge (per unit area) induced by the wall. Notice that in Eq. (15) B appears with its sign. This can be seen by our adding a small term that breaks the particle-hole symmetry (see Refs. 5, 6, and 14) in Eq. (5). The sign of B determines which zero modes are normalizable.[3] This charge is localized within a length scale $\xi \sim 1/m(\infty)$ from the wall. If a nonzero electric field $\mathbf{E}$ parallel to the wall is applied, say along the y direction, there is an *induced current in the x direction.* We can motivate this result by noting that if we go to a reference frame that moves along the x direction with velocity $v_x = cE/B$, there is an electric field $\mathbf{E} \sim (\mathbf{v}/c) \times \mathbf{B}$ (in the y direction) but a current in the x direction (charge flow),

$$J^x = (4e^2/h)E_y/4\pi. \tag{16}$$

These "quasi Hall currents" (or, more precisely, Chern-Simons currents) do not depend on the magnetic field. For $B = 0$, Eq. (16) gives the *abnormal-parity contribution* to the current induced by a *weak localized* electric field. This expression can be computed in perturbation theory.[6,7,10] Indeed, notice that Eq. (16) *does not* depend on the sign of B because Q in Eq. (15) changes sign with B. This is *unlike* the ordinary Hall effect where Eq. (16) would contain a factor of $\mathrm{sgn}(B)$. These Chern-Simons currents arise from the properties of the "Dirac spin" of the solution given by Eqs. (10) and (11).[6] In fact this suggests an interesting way for detection of these abnormal currents with the same experimental settings as in the Hall effect. If we consider crossed electric and magnetic fields, $J_{\text{C-S}}$ *does not change sign when* $B \to -B$, *unlike the Hall currents.* Note that the charge and current [Eqs. (15) and (16)] are components of a four-vector. It can be shown that this result is a generalization of the Callan-Harvey formula for the case of a scalar domain wall in 3+1 dimensions.[10] The sign of the induced charge Q and of the current is determined by the precise way that the Fermi sea is filled: The sign in Eq. (15) is minus (plus) for a filled (empty) zero mode. Thus our results predict that in a PbTe crystal with an antiphase boundary there is an induced charge per unit wall area (in the presence of a magnetic field), given by Eq. (15), and an odd-parity current [Eq. (16)] perpendicular to the electric field (even in the limit $B \to 0$).

Finally some remarks about degeneracy-lifting perturbations. The first example is a Zeeman term. It can be shown that this term produces a (very small) splitting of the zero modes thus canceling the effect. This can be compensated by the addition of extra electrons (doping). Some PbTe-type narrow-gap semiconductors exhibit Peierls distortions of various types. A Peierls distortion along the (111) axis can be shown to break particle-hole symmetry. The result is that the zero mode is either lowered or raised depending on which Peierls ground state the system is. This has either all zero modes empty or occupied. Still there are other more complicated cases.[14]

We wish to thank M. Stone for very useful comments. This work was supported in part by National Science Foundation Grant No. DMR84-15063 and U.S. Department of Energy Contract No. DE-AC03-76SF00515.

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