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# Condensed-Matter Simulation of a Three-Dimensional Anomaly

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A condensed-matter analog of $(2+1)$-dimensional electrodynamics is constructed, and the consequences of a recently discovered anomaly in such systems are discussed.

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Recently, new anomalous phenomena in $(2+1)$-dimensional systems of fermions and gauge fields have received much attention.[1-8] The associated fermion zero modes, induced currents of abnormal parity, unusual quantum numbers, and fractional statistics are interesting manifestations of the role of topological structures in quantum physics. Some of these, fractional charge and statistics in particular, are relevant to the understanding of the quantized Hall effect,[9] which appears in planar systems of nonrelativistic electrons. However, relativistic $(2+1)$-dimensional gauge theories still lack a realistic physical setting. The purpose of this Letter is to point out one such realization and to discuss the consequences of anomalies there.

In the lattice formulation of gauge theories on even-dimensional space-times the axial anomaly can be understood as an external field-induced level shift.[10] Recently, on this basis, the formal similarity of fermions in lattice gauge theories and the tight-binding description of electrons in crystals has been used to propose a condensed-matter analog of the $(3+1)$-dimensional axial anomaly.[11] In a hypothetical, parity-noninvariant, gapless semiconductor the electron energy bands exhibit degeneracy points, i.e., points on the Fermi surface where the conduction and valence bands intersect. The low-energy electron dynamics are described by linearizing their spectrum about the degeneracy points and are thus modeled by relativistic Weyl fermions. It is a general theorem that these must occur in right- and left-handed pairs.[12] In the presence of parallel external electric and magnetic fields the axial anomaly effects a transfer of electrons between the right- and left-handed degeneracy points, observable as a strong longitudinal magnetoconductance.

In the following we shall develop a similar condensed-matter analog of $(2+1)$-dimensional electrodynamics. We consider the tight-binding description of electrons on a planar, honeycomb lattice. The band structure exhibits two degeneracy points per Brillouin zone and the low-energy behavior is obtained in the continuum limit where two species of relativistic $(2+1)$-dimensional fermions emerge. Then, in accordance with general considerations, external magnetic fields induce zero modes in the electron energy spectrum, and the resulting degenerate ground states are charged. We shall suggest scenarios where these induced charges may be observed.

The model considered here has been used extensively to study the electromagnetic properties of graphite.[13] Graphite is a semimetal which to a first approximation is composed of independent layers of carbon atoms. Each layer forms a honeycomb lattice with one valence electron per atomic site. In the planar material, the existence of two degeneracy points per Brillouin zone is a general consequence of the lattice symmetries.[14] Here, we shall present a simple dynamical model where this degeneracy is explicit. In three-dimensional graphite, interplanar interactions break the symmetry,[15] and this model may not be strictly applicable there. However, there may be various types of intercalated or exfoliated graphite where the interplanar coupling is negligible. Furthermore, it may be possible to fabricate a graphite monolayer where the effects which we describe would be observable.

Before we present the details of our model let us review the salient features of three-dimensional electrodynamics. On odd-dimensional space-times chirality is absent (there is no analog of $\gamma^5$) and conservation laws for fermionic currents are not anomalous. However, a new phenomenon of this type is known to arise.[2-7] For each species of fermions, external gauge fields induce a current of abnormal parity in the ground state. For example, consider a fermion coupled to a U(1) gauge field in $(2+1)$-dimensions with Lagrangian

$$L(x)=\bar{\psi}(x)(i\gamma^\mu D_\mu - m)\psi(x) \quad , \tag{1}$$

where $\gamma^\mu=(\sigma^3, i\sigma^1, i\sigma^2)$ ($\sigma^i$ are the Pauli matrices) and $D_\mu=\partial_\mu - ieA_\mu$. The induced current is

$$j^\mu(x)=(e/8\pi)\epsilon^{\mu\nu\lambda}F_{\nu\lambda}(x)\,\mathrm{sgn}(m)+\dots . \tag{2}$$

Corrections to (2) are of higher orders in derivatives of $F_{\mu\nu}=\partial_\mu A_\nu - \partial_\nu A_\mu$ and (2) gives the induced electric charge $Q=\int d^2x\, j^0(x)=e\Phi/2\,\mathrm{sgn}(m)$ exactly,[2] where $\Phi=2\pi^{-1}\int d^2x\, B(x)$ is the magnetic flux. The mass term in (1) violates parity which is defined as the reflection of one spatial coordinate:

$$A_{0,2}(x_1,x_2,t)\rightarrow A_{0,2}(-x_1,x_2,t);$$
$$A_1(x_1,x_2,t)\rightarrow -A_1(-x_1,x_2,t);$$
$$\psi(x_1,x_2,t)\rightarrow \sigma^1\psi(-x_1,x_2,t).$$

When $m\rightarrow 0$, (1) is formally invariant under this transformation. However, the current (2) retains its parity-noninvariant contribution with an ambiguous sign.

This sign anomaly of the massless limit has its origin in the existence of zero-energy bound states of the relevant Dirac Hamiltonian,[5] $H=-i\gamma^0\vec{\gamma}\cdot\vec{D}$. In a static background magnetic field ($A_0=0$, $\dot{A}_i=0$) with quantized flux, $|\Phi|=n$, the spatial manifold can be compactified to $S^2$ (rather than $R^2$),[16,17] the spectrum of $H$ is discrete, and index theorems[16,18] (or an explicit construction[5]) indicate $n$ zero modes. The ground state of the quantum systems is $(n+1)$-fold degenerate with induced vacuum charges $Q=-(e/2)|\Phi|, -(e/2)|\Phi|+e, \dots, (e/2)|\Phi|$.[19]

Consider the planar honeycomb lattice depicted in Fig. 1. The Bravais lattice is triangular and the unit cell contains two sites, which we denote type A and type B. The type A sites are generated by linear combinations of the basis vectors $\vec{a}_1=(\frac{1}{2}\sqrt{3}, -\frac{1}{2})a$; $\vec{a}_2=(0,1)a$ (where $a$ is the lattice spacing), with integer coefficients, $\vec{A}(n_1n_2)=n_1\vec{a}_1+n_2\vec{a}_2$. The sublattices are connected by the vectors $\vec{b}_1=(1/2\sqrt{3},\frac{1}{2})a$; $\vec{b}_2=(1/2\sqrt{3},-\frac{1}{2})a$; $\vec{b}_3=(-1/\sqrt{3},0)a$, and the type B sites are generated by $\vec{B}(m_1m_2)=m_1\vec{a}_1+m_2\vec{a}_2+\vec{b}_1$. The reciprocal-lattice basis vectors are $\vec{R}_1=(4\pi/\sqrt{3}a)(1,0)$; $\vec{R}_2=(4\pi/\sqrt{3}a)(\frac{1}{2},\frac{1}{2}\sqrt{3})$ and the Brillouin zone, $\Omega_B$, is a hexagon in momentum space with opposite sides identified (see Fig. 2).

The graphite lattice is monatomic with the sites occupied by carbon atoms. We consider a slightly more general diatomic system by assuming that sites A and B are occupied by distinct types of atoms. We parametrize the difference of energies of electrons localized on A and B by $\beta$. An example of a layered diatomic material described by this

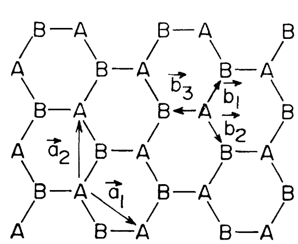


FIG. 1. The honeycomb lattice as a superposition of two triangular sublattices. The basis vectors are $\vec{a}_1=(\sqrt{3}/2,-\frac{1}{2})a$; $\vec{a}_2=(0,1)a$ and the sublattices are connected by $\vec{b}_1=(1/2\sqrt{3},\frac{1}{2})a$; $\vec{b}_2=(1/2\sqrt{3},-\frac{1}{2})a$; $\vec{b}_3=(-1/\sqrt{3},0)a$.

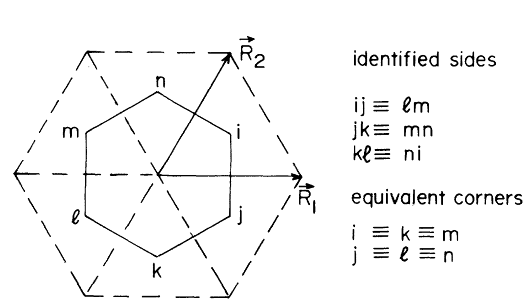


FIG. 2. The Brillouin zone. The reciprocal-lattice basis vectors are $\vec{R}_1=(4\pi/\sqrt{3}a)(1,0)$; $\vec{R}_2=(4\pi/\sqrt{3}a)\times(\frac{1}{2},\frac{1}{2}\sqrt{3})$. The degeneracy points occur at the corners, *ijklmn*, of the Brillouin zone. Two of these are inequivalent; we have chosen $\vec{q}_1=(4\pi/\sqrt{3}a)(\frac{1}{2},1/2\sqrt{3})$ at point *i* and $\vec{q}_2=-\vec{q}_1$ at point *l*.

lattice is boron nitride.[20] The graphite model is regained by setting $\beta$ to zero.

In the tight-binding approximation and where only nearest-neighbor interactions are retained, the Hamiltonian is

$$H=\alpha\sum_{\vec{A},i}[U^\dagger(\vec{A})V(\vec{A}+\vec{b}_i)+V^\dagger(\vec{A}+\vec{b}_i)U(\vec{A})]+\beta\sum_{\vec{A}}[U^\dagger(\vec{A})U(\vec{A})-V^\dagger(\vec{A}+\vec{b}_1)V(\vec{A}+\vec{b}_1)]. \quad (3)$$

Here $U^\dagger$ and $U$ ($V^\dagger$ and $V$) are the creation and destruction operators for electrons localized on sites A (B), respectively. The hopping parameter $\alpha$ is related to the probability amplitude for electron transfer between neighboring sites. For the moment, we ignore the electron spin. Using the Fourier transform

$$U(\vec{A})=\int_{\Omega_B}\frac{d^2k}{(2\pi)^2}e^{i\vec{k}\cdot\vec{A}}U(\vec{k}),\quad V(\vec{B})=\int_{\Omega_B}\frac{d^2k}{(2\pi)^2}e^{i\vec{k}\cdot\vec{B}}V(\vec{k})$$

in (3) results in

$$H=\int_{\Omega_B}\frac{d^2k}{(2\pi)^2}[U^\dagger(\vec{k}),V^\dagger(\vec{k})]\begin{bmatrix}\beta & \alpha(e^{i\vec{k}\cdot\vec{b}_1}+e^{i\vec{k}\cdot\vec{b}_2}+e^{i\vec{k}\cdot\vec{b}_3})\\ \alpha(e^{-i\vec{k}\cdot\vec{b}_1}+e^{-i\vec{k}\cdot\vec{b}_2}+e^{-i\vec{k}\cdot\vec{b}_3}) & -\beta\end{bmatrix}\begin{bmatrix}U(\vec{k})\\ V(\vec{k})\end{bmatrix}.$$

The energy eigenvalues are $E(k)=\pm(\beta^2+\alpha^2|e^{i\vec{k}\cdot\vec{b}_1}+e^{i\vec{k}\cdot\vec{b}_2}+e^{i\vec{k}\cdot\vec{b}_3}|^2)^{1/2}$. With one electron per site (one electron per unit cell per spin degree of freedom), the negative-energy states (valence band) are filled and the positive-energy states (conduction band) are empty. The separation of the conduction and valence bands is minimal at the zeros of $\exp(i\vec{k}\cdot\vec{b}_1)+\exp(i\vec{k}\cdot\vec{b}_2)+\exp(i\vec{k}\cdot\vec{b}_3)$. These occur at $\vec{q}_1=(4\pi/\sqrt{3}a)\times(\frac{1}{2},1/2\sqrt{3})$, $\vec{q}_2=-\vec{q}_1$, and all other equivalent points, which are the corners of the Brillouin zone (*ijklmn* in Fig. 2). In the continuum (low energy) limit ($a\to 0$), only electron states near $\vec{q}_1$ and $\vec{q}_2$ participate in the dynamics. We obtain two species of fermions:

$$\psi_1(\vec{k})=\tfrac{1}{2}\alpha a\sqrt{3}\exp(-i\tfrac{1}{3}\pi\sigma^3)\begin{bmatrix}U(\vec{k}-\vec{q}_1)\\ V(\vec{k}-\vec{q}_1)\end{bmatrix},\quad \psi_2(\vec{k})=\tfrac{1}{2}\alpha a\sqrt{3}\exp(-i\tfrac{1}{3}\pi\sigma^3)\sigma^1\begin{bmatrix}U(\vec{k}+\vec{q}_1)\\ V(\vec{k}+\vec{q}_1)\end{bmatrix}, \quad (4)$$

with Hamiltonian

$$H=\int[d^2k/(2\pi)^2][\bar{\psi}_1(\vec{k})(\vec{\gamma}\cdot\vec{k}+m)\psi_1(\vec{k})+\bar{\psi}_2(\vec{k})(\vec{\gamma}\cdot\vec{k}-m)\psi_2(\vec{k})],$$

where $m=2\beta/\sqrt{3}\alpha a$. In coordinate space,

$$H=\int[d^2x/(2\pi)^2][\bar{\psi}_1(x)(\vec{i}\gamma\cdot\vec{D}+m)\psi_1(x)+\bar{\psi}_2(x)(\vec{i}\gamma\cdot\vec{D}-m)\psi_2(x)], \quad (5)$$

where we have assumed that the interaction with the electromagnetic field proceeds through minimal coupling.

The Hamiltonian in (5) is invariant under parity when the fermions $\psi_1$ and $\psi_2$ transform into each other: $\psi_1(x_1,x_2,t)\to\sigma^1\psi_2(-x_1,x_2,t)$; $\psi_2(x_1,x_2,t)\to\sigma^1\psi_1(-x_1,x_2,t)$. Furthermore, it has the conjugation symmetry $\psi_1\to\sigma^3\psi_2$, $\psi_2\to\sigma_3\psi_1$, $H\to -H$. The separately conserved induced currents are

$$j_1^\mu(x)=\langle\tfrac{1}{2}[\bar{\psi}_1,\gamma^\mu\psi_1]\rangle =(e/4\pi)\epsilon^{\mu\nu\lambda}F_{\nu\lambda}(x)\,\mathrm{sgn}(m)+\cdots,$$

and

$$j_2^\mu(x)=\langle\tfrac{1}{2}[\bar{\psi}_2,\gamma^\mu\psi_2]\rangle =-(e/4\pi)\epsilon^{\mu\nu\lambda}F_{\nu\lambda}(x)\,\mathrm{sgn}(m)+\cdots,$$

where we have included a factor of 2 for the spin degeneracy. Therefore, because of the fermion doubling, the electric current $j_+^\mu=j_1^\mu+j_2^\mu$ vanishes. The odd combination is nonzero:

$$j_-^\mu=j_1^\mu-j_2^\mu =(e/2\pi)\epsilon^{\mu\nu\lambda}F_{\nu\lambda}(x)\,\mathrm{sgn}(m)+\cdots.$$

However, it would couple to an unphysical external field of abnormal parity and is therefore not directly observable.

In the massless limit $\beta\to 0$ or $m\to 0$ we recover the graphite model. There the general considerations imply that in an external magnetic field with flux $|\Psi|=n$, there are $2n$ zero-energy modes. If we take the electron spin into account, each of these bound states is a spin doublet. The ground state is then $(4n+1)$-fold degenerate, the charges of these states being $Q=-2e|\Phi|, -2e|\Phi|+e, \ldots, 2e|\Phi|$.

The spinless state (all spins paired) with charge $Q=+(-)2e|\Phi|$ is easily obtained by the introduction of a small positive (negative) chemical potential which guarantees that all zero-energy levels are occupied (unoccupied). Alternatively, if the electrons are subject to the Zeeman interaction which has the effect of raising the energy of those whose spins are aligned parallel with a uniform external magnetic field and of lowering the energy of those antialigned, the system would be uncharged but would have $2n$ unpaired spins.

The latter scenario would be observable as an anisotropic electron spin-resonance amplitude. The Zeeman splitting of the energy levels is approximately independent of the direction of the external field. However, the flux through the plane of the system (and therefore the number of zero modes) is proportional to the sine of the angle $\theta$ between the plane and the external field. The number of unpaired spins per unit area is therefore equal to $4\pi B \sin\theta$. The angle dependence of the electron spin-resonance amplitude would be direct evidence for the vacuum degeneracy. Observation of this effect in a real material such as planar graphite would be an interesting confirmation of the phenomena which we have described.

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[1]S. Deser, R. Jackiw, and S. Templeton, Phys. Rev. Lett. **48**, 372 (1982), and Ann. Phys. (N.Y.) **140**, 975 (1982).

[2]I. Affleck, J. Harvey, and E. Witten, Nucl. Phys. **B206**, 413 (1982).

[3]A. J. Niemi and G. W. Semenoff, Phys. Rev. Lett. **51**, 2077 (1983).

[4]A. N. Redlich, Phys. Rev. Lett. **52**, 1 (1984), and Phys. Rev. D **29**, 2366 (1984).

[5]R. Jackiw, Phys. Rev. D **29**, 2375 (1984).

[6]J. Lott, to be published.

[7]L. Alvarez-Gaumé, S. Della Pietra, and G. Moore, to be published.

[8]F. Wilczek, Phys. Rev. Lett. **49**, 957 (1982); F. Wilczek and A. Zee, to be published; Y.-S. Wu, Phys. Rev. Lett. **52**, 2103 (1984).

[9]B. I. Halperin, Phys. Rev. Lett. **52**, 1583 (1984); F. Wilczek and A. Zee, unpublished; R. Tao and Y.-S. Wu, to be published.

[10]J. Ambjorn, J. Greensite, and C. Peterson, Nucl. Phys. **B221**, 381 (1983).

[11]H. B. Nielsen and M. Ninomiya, Phys. Lett. **130B**, 389 (1983).

[12]H. B. Nielsen and M. Ninomiya, Nucl. Phys. **B185**, 20 (1981), and **B193**, 173 (1981).

[13]P. K. Wallace, Phys. Rev. **71**, 622 (1947); for reviews, see R. R. Haering and S. Morozoeski, Prog. Semicond. **5**, 274 (1960); J. Calloway, *Energy Band Theory* (Academic, New York, 1964); F. Bassani and G. Pastori Parravicini, *Electronic States and Optical Transitions in Solids* (Pergamon, New York, 1975); F. Kelley, *Physics of Graphite* (Elsevier, New York, 1981).

[14]W. M. Lomer, Proc. Roy. Soc. London, Ser. A **277**, 330 (1960).

[15]R. R. Haering and P. R. Wallace, J. Phys. Chem. Solids **3**, 253 (1957); J. W. McClure, Phys. Rev. **104**, 666 (1956), and **119**, 606 (1960); Ref. 14.

[16]M. Ansourian, Phys. Lett. **70B**, 301 (1977); H. Romer and B. Schroer, Phys. Lett. **71B**, 182 (1977).

[17]For some analysis on the open space $R^2$, see Ref. 3 and A. J. Niemi and G. W. Semenoff, Phys. Rev. D **30**, 809 (1984).

[18]M. Atiyah and I. Singer, Ann. Math. **87**, 484 (1964); for a review, see T. Eguchi, R. Gilkey, and A. Hanson, Phys. Rep. **66C**, 213 (1980).

[19]This is a particular example of the general relationship between fermion zero modes and fractional charges seen in many systems where fermions interact with certain topological background fields. See R. Jackiw and C. Rebbi, Phys. Rev. D **13**, 3398 (1976); Refs. 3 and 5; and, for reviews, R. Jackiw, Comments Nucl. Part. Phys. **13**, 15, 141 (1984); A. J. Niemi and G. W. Semenoff, to be published.

[20]F. Bassani *et al.*, Ref. 13.