Topological piezoelectric effect and parity anomaly in nodal line semimetals

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Lattice deformations act on the low-energy excitations of Dirac materials as effective axial vector fields. This allows to directly detect quantum anomalies of Dirac materials via the response to axial gauge fields. We investigate the parity anomaly in Dirac nodal line semimetals induced by lattice vibrations, and establish a topological Hall effect; i.e., periodic lattice deformations generate topological Hall currents that are transverse to the deformation field. The currents induced by this piezoelectric effect are dissipationless and their magnitude is completely determined by the length of the nodal ring, leading to a semi-quantized transport coefficient. Our theoretical proposal can be experimentally realized in various nodal line semimetals, such as CaAgP and Ca3P2.

Introduction.— Over the last few years a number of new types of topological semimetals have been discovered [1][4]. Among them are Weyl semimetals and Dirac semimetals with point nodes, around which the bands have linear dispersion in all directions. The low-energy physics of these point node semimetals is described by relativistic field theories with quantum anomalies, i.e., by quantum field theories that break symmetries of the classical action. For instance, two-dimensional Dirac materials, such as graphene, are described by quantum field theories with parity anomalies, that break space-time inversion symmetry [8][9]. The low-energy theories of Weyl semimetals, on the other hand, exhibit chiral anomalies, which violate conservation of axial charge [10][14]. The chiral anomaly in Weyl semimetals give rise to numerous experimental phenomena [15][19], for example, negative magnetoresistance, which has been observed in recent experiments [19][20]. Lattice strain, which generates axial magnetic fields, can also be used to probe the chiral anomaly [21][34].

At the same time, recent research has focused on Dirac materials with line nodes [35][39]. These nodal-line semimetals (NLSMs) can be viewed as three-dimensional generalizations of graphene. They exhibit Dirac band crossings along a one-dimensional line in a three-dimensional Brillouin zone, with low-energy excitations that are linearly dispersing in the two directions perpendicular to the band-crossing line. NLSMs possess a number of interesting properties, e.g., topological surface charges, drumhead surface states [43][44], and quasitopological electromagnetic responses [45][46]. The low-energy excitations around the nodal ring of these semimetals are described by one-parameter families of (2+1)-dimensional quantum field theories with parity anomalies [47]. That is, the electromagnetic responses of these nodal rings are given by Chern-Simons actions, which break parity symmetry. These Chern-Simons terms lead to transverse Hall effects, where electrons from opposite sides of the nodal ring flow to opposite surfaces, when an electric field is applied [47].

Unfortunately, due to time-reversal symmetry, the total current generated by the Chern-Simons action vanishes, once the sum over all momenta is taken. Therefore, the electric-field induced Hall currents can only be measured by special devices, that filter electrons based on their momenta [47].

In this letter, we propose to use pseudo electric fields, induced by lattice vibrations, to probe the parity anomaly of NLSMs. As opposed to external electric fields, pseudo electric fields are axial, as they couple with opposite sign to electrons with opposite momenta. This permits to directly probe the parity anomaly of NLSMs, via the response to axial electric fields. We derive a low-energy description of NLSMs in the presence of strain, and show that periodic lattice deformations generate a topological piezoelectric effect (TPEE), which originates from the parity anomaly. This piezoelectric effect manifests itself by dissipationless Hall currents that are transverse to the deformation field. We show that the TPEE can be interpreted as a polarization current and that it has a semi-quantized transport coefficient, given by the length of the nodal ring. Furthermore, we discuss experimental considerations for the observation of the TPEE in the NLSM materials CaAgP and Ca3P2.

Model.— First, we introduce a lattice model for a NLSM with a single nodal ring, and discuss its topological properties. We consider the following tight-binding Hamiltonian on the cubic lattice

\[
H(p) = t [2 + \cos p_0 a - \cos p_z a - \cos p_y a - \cos p_z a] \tau_z + v \sin p_z a \tau_y + \Delta \tau_x,
\]

where \(\tau_i\) (i = 1, 2, 3) are Pauli matrices acting in orbital space. For simplicity, we assume \(t, v, p_0 > 0\). To discuss the parity anomaly and the electric polarization, we have introduced a small parity-breaking term \(\Delta \tau_z\). In the absence of \(\Delta \tau_z\), the lattice Hamiltonian is parity-time (PT) symmetric with the \(PT\) operator \(PT = \tau_z K\). This tight-binding Hamiltonian describes the low-energy dispersion near the Fermi level of CaAgP and Ca3P2 [36][33]. The symmetry-breaking term \(\Delta \tau_z\) can be induced by applying uniaxial pressure, or an electric field [44].

In the absence of \(\Delta \tau_z\), Hamiltonian [1] exhibits a nodal ring within the \(p_z = 0\) plane, centered around \(\Gamma\). This
The subsystem is given by the Zak’s phase \[ \nu[S^1] \] which is an \( \mathbb{Z}_2 \) invariant:

\[
\nu[S^1] = \frac{1}{\pi} \sum_{\alpha \in \text{occ. states}} \int_{S^1} dp \cdot A_{\alpha}^\alpha(p) \mod 2, \tag{2}
\]

where the integration path is along the closed loop \( S^1 \). Here, \( A_{\alpha}^\beta(p) = i \langle u_\alpha(p) | \partial_p | u_\beta(p) \rangle \) and \( | u_\alpha(p) \rangle \) are the Berry connection and the Bloch eigenstates of Eq. (1), respectively. \( \mathcal{PT} \) symmetry restricts \( \nu[S^1] \) to the values \( \nu[S^1] = 0, 1 \). When the loop \( S^1 \) encircles the nodal ring, we obtain \( \nu[S^1] = 1 \), otherwise \( \nu[S^1] = 0 \).

The topological protection of the nodal ring is linked to a bulk electric polarization. To see this, let us decompose the three-dimensional Hamiltonian (1) into one-dimensional subsystems parametrized by the inplane momenta \( p_\perp = (p_x, p_y) \). The electric polarization of each subsystem is given by Zak’s phase [43],

\[
P_z(p_\perp) = \sum_{\alpha \in \text{occ. states}} \int_{-\pi}^{\pi} dp_z \frac{1}{2\pi} A_{z}^\alpha(p) = 0, \quad \frac{1}{2}, \tag{3}
\]

and the total polarization is the summation of these phases over the inplane momenta

\[
P_z = \int \frac{dp_\perp}{(2\pi)^2} P_z(p_\perp). \tag{4}
\]

From Eqs. (2) and (3), we find that the Zak’s phase is \( \frac{1}{2} \) for a region of inplane momenta \( p_\perp \) that is bounded by the nodal ring. By the bulk-boundary correspondence [44], this leads to midgap surface states at the (001) face of the NLSM, whose fillings determine the surface charge. Due to \( \mathcal{PT} \) symmetry, the surface states at the top and bottom (001) faces are degenerate, thus the electric polarization is determined only up to a multiple of the elementary charge. To unambiguously determine the bulk polarization, it is necessary to include an infinitesimal \( \mathcal{PT} \) symmetry breaking term \( \Delta \tau_x \), which opens a bulk gap and removes the degeneracy of the midgap surface states. With the inclusion of \( \Delta \tau_x \), we find that the bulk polarization is semi-quantized and given by [45],

\[
P_z = \frac{S}{8\pi^2} \text{sign}(\Delta), \tag{5}
\]

where \( S \) is the area encircled by the nodal ring projected onto the surface Brillouin Zone.

**Parity anomaly and Chern-Simons action.** — Next, we use a family of (2+1)-dimensional quantum field theories to derive the topological responses due to external and pseudo electromagnetic fields. For small \( p \), Eq. (1) reduces to the low-energy continuum Hamiltonian

\[
H_{\text{eff}}(p) = \frac{p^2 - p_z^2 + \lambda p_z}{2m} \tau_y + \Delta \tau_x, \tag{6}
\]

where \( 1/(2m) = ta^2/2 \) and \( \lambda = v\alpha \). Eq. (6) has rotational symmetry around the \( p_z \) axis. Thus, we introduce cylindrical coordinates \( (p_r, \phi, p_z) \) with \( p_r \in (-\infty, \infty), \) and \( \phi \in [0, \pi], \) see Fig. 1. With these cylindrical coordinates, we can decompose the three-dimensional system into a family of two-dimensional subsystems labeled by the azimuth angle \( \phi \in [0, \pi] \). Each of these subsystems contains two Dirac points that are related by time-reversal symmetry, and which have opposite sign of Berry curvature \( \chi = \text{sign}(\Delta) = \pm 1 \).

Each subsystem, labeled by \( \phi \), is described by the following (2+1)-dimensional quantum field theory

\[
S_{\phi} = \bigoplus_{\chi = \pm 1} S_{\phi, \chi} \tag{7}
\]

\[
S_{\phi, \chi} = \int d^2 x \, dt \, \overline{\psi} \left[ i\chi \gamma^\mu \left( \partial_\mu + iA_\mu + i\chi A_5^\mu + \Delta \right) \right] \psi,
\]

where \( \psi \) is a two-component Dirac spinor, \( \overline{\psi} = \psi^\dagger \gamma_0 \), \( \{ \gamma_\mu, \gamma_\nu \} = i \eta_{\mu\nu} \), and \( \eta_{\mu\nu} = \text{diag}(1, -1, -1) \). The Dirac spinors interact with the total gauge field \( A_\mu^5 = A_\mu + \chi A_5^\mu \), which contains both an external gauge field \( A_\mu \) and an axial gauge field \( A_5^\mu \), respectively. We note that the axial gauge field couples with opposite sign \( \chi \) to the two Dirac points of the subsystem. The physical origin of \( A_5^\mu \) due to lattice strain will be discussed later. Upon regularization [4], we obtain from Eq. (8) the parity breaking Chern-Simons term

\[
S_{\text{CS}}^{\phi, \chi} = \frac{\chi}{4\pi} \int d^2 x \, dt \, \epsilon^{\mu\nu\lambda} A_\mu^5 \partial_\nu A_\lambda^5, \tag{8}
\]

which is a manifestation of the parity anomaly. Varying the Chern-Simons action with respect to \( A_\mu \), gives the anomalous transverse current

\[
j_{\mu, \chi} = -\frac{\delta S_{\text{CS}}^{\phi, \chi}}{\delta A_\mu} = \frac{\chi}{4\pi} \epsilon^{\mu\nu\lambda} (\partial_\nu A_\lambda + \chi \partial_\nu A_5^\lambda), \tag{9}
\]
for a single Dirac point with chirality $\chi$ in subsystem $\phi$. We observe that transverse currents induced by external electromagnetic fields cancel out, since contributions from opposite sides of the nodal ring have opposite sign $\chi = \pm 1$. Currents induced by axial gauge fields, however, do not cancel, since they have the same sign everywhere along the nodal ring. This remarkable feature originates from the axial nature of the strain-induced gauge field $A_5^\mu$, which couples oppositely to Dirac fermions with opposite momenta.

**Strain-induced axial gauge field.**—We now discuss the physical origin of the axial gauge field. The basic idea is to incorporate lattice strain into the tight-binding model [1], which acts on the low-energy excitations as effective gauge fields. Strain shifts the lattice sites $R$ by the displacement vector $u(R)$, as $R + u(R)$, thereby modifying and introducing new overlaps between atomic orbitals. In our tight binding model this changes the hopping parameters as [51 52]

$$t(a_x)_{\tau_z} \simeq t(1 - u_{xx})_{\tau_z} + ivu_{xz}t_y, \quad (10a)$$

$$t(a_y)_{\tau_z} \simeq t(1 - u_{yy})_{\tau_z} + ivu_{yz}t_y, \quad (10b)$$

$$t(a_z)_{\tau_z} \simeq t(1 - u_{zz})_{\tau_z}, \quad (10c)$$

$$iv(a_z)_{\tau_y} \simeq iv(1 - u_{zz})_{\tau_y} + t \sum_{i \neq z} u_{zi}t_z, \quad (10d)$$

where $t(a_\mu)(\mu = x, y, z)$ represents the hopping amplitudes along the bond direction $a_\mu$, and $u_{\mu\nu} = (\partial_\mu u_\nu(R) + \partial_\nu u_\mu(R))/2$ is the symmetrized strain tensor. The first terms in Eqs. (10) describe changes in the hopping amplitudes between two like orbitals, when the bond lengths are modified by strain. The second terms originate from new hopping processes between different orbitals, which are symmetry forbidden in the unstrained lattice. In the following, we focus on the gauge fields induced by the $u_{\mu\nu}$ components of the stress tensor, as these are the ones that probe the parity anomaly. The other components of $u_{\mu\nu}$ only renormalize the Fermi velocity, which is not important for our purpose. Using Eq. (10) we find that this lattice strain generates additional terms in the tight-binding Hamiltonian [1], $H(p) \rightarrow H(p) + \delta H(p)$, which are of the form [53]

$$\delta H(p) \simeq -tu_{xz} \cos p_xa \tau_z$$

$$+v(u_{xz} \sin p_xa + u_{yz} \sin p_ya)t_y, \quad (11)$$

These modifications change the low-energy Hamiltonian [6] to

$$H_{\text{eff}}(p) + \delta H_{\text{eff}}(p) \simeq v_F (q_t - A_5^z) \tau_z + \lambda (p_z - A_5^z(\psi)) \tau_y + \Delta \tau_x, \quad (12a)$$

with the pseudo gauge potentials

$$A_5^z = u_{xz}/(p_0a^2), \quad (12b)$$

$$A_5^z(\psi) = \sum_i f_i(\psi)A_5^z \simeq -v_0 (u_{xz} \cos \psi + u_{yz} \sin \psi),$$

along the $r$- and $z$-directions, respectively, where $f_z(\psi) = p_0 \cos \psi$, $f_y(\psi) = p_0 \sin \psi$, and $A_5^{z0} = -u_{xz}$ ($i = x, y$). Here, we have introduced the Fermi velocity $v_F = p_0/m$, the radial momentum $q_r = p_r - p_0$, and the cylindrical coordinates $(p_r, p_z, \psi)$ with $p_r \in [0, \infty)$, $p_z \in (-\infty, \infty)$, $\psi \in [0, 2\pi]$.

We conclude that in NLSMs with a nodal ring in the $p_z = 0$ plane, the strain field components $u_{\mu\nu}$ act on the low-energy excitations like effective gauge potentials. Interestingly, these effective gauge potentials are axial, since they couple with opposite sign to the excitations at opposite sides of the nodal ring, i.e., at $(p_0, 0, \psi)$ and $(p_0, 0, \psi + \pi)$. From Eq. (12), we see that $A_5^z$ concentrically shrinks or expands the nodal ring, while $A_5^{z0}$ tilts the nodal ring out of the $p_z = 0$ plane, see Figs. [2]a and [2]b, respectively.

If we consider time-dependent lattice strain, i.e., lattice vibrations, we can also generate axial electric fields. That is, the time dependence of the strain tensor $u_{\mu\nu}(t)$ produces axial electric fields via

$$E_5^x = -\frac{\partial A_5^x}{\partial t}, \quad E_5^y = -\frac{\partial A_5^y}{\partial t},$$

(13)

where the axial electric fields $E_5^{x, y}$ are defined by the angular independent parts of the axial vector potentials, and $f_z(\psi)$ are absorbed into the axial charge coupling constants.

**Topological piezoelectric effect.**—Next, we demonstrate that axial electric fields in NLSMs induce net topological currents that flow in the direction perpendicular to the axial fields. For that purpose we use linear response theory to compute the axial conductivity tensors $\tilde{\sigma}_{\mu\nu}(\omega)$ and $\tilde{\sigma}_{x\mu}(\omega)$, which are defined as

$$\langle \hat{j}_{\mu}(\omega) \rangle = \tilde{\sigma}_{\mu\nu}(\omega)E_5^\nu(\omega) + \tilde{\sigma}_{x\mu}(\omega)E_5^{x, y}(\omega),$$

(14)

with the current density operator $\hat{j}$. By use of Kubo’s formula we compute the axial Hall conductivities $\tilde{\sigma}_{xz}(T, \omega)$ and $\tilde{\sigma}_{zz}(T, \omega)$ [54]. In the DC limit $\omega \rightarrow 0$, they are given by

$$\tilde{\sigma}_{xz}^{\text{DC}}(T) = -\frac{1}{V} \sum_{p, \alpha} f(\epsilon_p^\alpha)B_{xz}^{\alpha}(p),$$

(15a)

$$\tilde{\sigma}_{zz}^{\text{DC}}(T) = -\frac{1}{V} \sum_{p, \alpha} f(\epsilon_p^\alpha)p_0 \cos \phi B_{zz}^{\alpha}(p),$$

(15b)

where $\epsilon_p^\alpha$, $f(\epsilon_p^\alpha)$ and $B_{\mu\nu}^\alpha(p) = -2\text{Im}(\partial_{p_\mu}u_\alpha(p)\partial_{p_\nu}u_\alpha(p))$ are the energy of the Bloch electrons, the Fermi function, and the Berry curvature, respectively.

Thus, it follows that axial electric fields produce transverse Hall currents, whose magnitude is determined by the Berry curvature. These Hall currents are perpendicular to both the axial electric field and the Berry curvature, see Figs. [2]b and [2]c. For instance, axial electric fields along the $r$ direction lead to electric currents in
the $z$ direction, since the direction of the Berry curvature is within the $p_z = 0$ plane. Similarly, axial electric fields along the $z$ direction produce currents in the $p_z = 0$ plane. Because the axial electric fields are generated by lattice vibrations, we refer to this type of Hall response as a topological piezoelectric effect.

Interestingly, in the low-frequency regime $|\omega/\Delta| \ll 1$, the axial Hall conductivities become semi-quantized, i.e., their magnitude depends only on the length of the nodal ring $L = 2\pi p_0$. That is, in the limit $|\omega/\Delta| \ll 1$ we find

$$\tilde{\sigma}^{DC}_{zr}(T = 0) \approx -\frac{L}{8\pi^2} \text{sign}(\Delta),$$

$$\tilde{\sigma}^{x,DC}_{zr}(T = 0) \approx \frac{L}{16\pi^2} \text{sign}(\Delta),$$

where $|\Delta/(v_F p_{\text{cut}})|$, $|\Delta/(\lambda p_{\text{cut}})| \ll 1$ is assumed, with some cut-off momentum $p_{\text{cut}}$. This is confirmed by numerical evaluations of $\tilde{\sigma}_{zr}(T = 0, \omega)$, see Fig. 3. We observe in Figs. 3(a) and 3(b) that the axial Hall conductivity asymptotically approaches its semi-quantized value for $\omega \to 0$, once $\Delta$ becomes sufficiently small and $p_{\text{cut}}$ sufficiently large, respectively. As displayed in the inset of Fig. 3(a) the semi-quantized value of the DC axial Hall conductivity scales linearly with the size of the nodal ring.

Before concluding, we show that the TPEE is related to the polarization current of NLSMs. As discussed above, the axial electric field $E^z_r(t)$ periodically shrinks and expands the nodal ring. This leads to a periodic fluctuation of the bulk electric polarization, which is determined by the size of the nodal ring. Hence, the axial electric field generates a polarization current, which according to Eq. (5), takes the form

$$j^\text{pol}_z = \frac{d P_z(t)}{d t} = \frac{1}{8\pi^2} \frac{d S(t)}{d t} \approx -\frac{L}{8\pi^2} \text{sign}(\Delta) E^z_r(t),$$

where $S(t) = \pi(p_0 + A^z_0(t))^2$ is the area of the nodal ring. Since Eq. (17) coincides with Eq. (16b), we conclude that the TPEE is linked to the polarization current of NLSMs and that its quantization arises from the semi-quantized electric polarization.

The proposed TPEE is testable in the materials CaAgP or Ca$_3$P$_2$, which exhibit a single nodal ring near the Fermi energy. In these materials rapid lattice vibrations can be generated using microwave radiation, which leads to an AC current via the TPEE. To estimate the magnitude of the current in Ca$_3$P$_2$, the relevant material parameters are $v_F = 2.72 \times 10^5$ m/s, $\lambda = 3.80 \times 10^5$ m/s, $p_0 = 0.206$ Å$^{-1}$, and $a = 8.26$ Å [3]. If the lattice is vibrating with frequency 100 MHz and amplitude 0.3% of $a$, and the parity breaking term is assumed to be $|\Delta/(v_F p_0)| = 0.001$, then the TPEE current is estimated to be about $j_z \approx 550$ mA/cm$^2$, which is experimentally detectable.

Conclusion.— We have shown that periodic strain fields lead to the TPEE, which manifests itself by dissipationless Hall currents, originating from the parity anomaly. While it would be of fundamental interest to observe the parity anomaly in NLSMs using lattice vibrations, the proposed TPEE could also be useful for future piezoelectric devices.

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FIG. 2: (a),(c) The axial gauge potential $A^z_r(t)$ changes the size of the nodal ring, while $A^z_r(t)$ tilts it out of plane, as indicated by the dashed lines. (b),(d) The strain induced currents $j^{\phi,x}$ (pink) are perpendicular to both the Berry curvature $B^z_r(p)$ (green) and the axial electric field $E^z$ (blue).
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[55] Here, we have also neglected the term $\nu u_2 \sin k_z \tau_y$, as it only renormalizes the hopping amplitude $\nu$.
[56] The details of the calculation are given in the supplemental materials.
Supplemental Materials

Derivation of Eq. (15)

Here, we summarize the derivation of Eq. (20a) and Eq. (20b).

To discuss the topological transport, we use the Bloch eigenbasis \( \{ |u_{\pm}(p)\rangle \} \) with
\[
H_{\text{eff}}(p)|u_{\pm}(p)\rangle = \epsilon_{p}^\pm |u_{\pm}(p)\rangle,
\]
\[
\epsilon_{p}^\pm = \pm \sqrt{v_{F}^{2}q_{r}^{2} + \lambda^{2}p_{z}^{2} + \Delta^{2}},
\]
and express the current density operator as
\[
\hat{j} = \sum_{p, \alpha = \pm} \partial_{p} \epsilon_{p}^\alpha \hat{c}_{p\alpha} \hat{c}_{p\alpha} + i \sum_{\alpha \neq \beta} (\epsilon_{p}^\alpha - \epsilon_{p}^\beta) \hat{A}_{p}^{\alpha, \beta}(p) \hat{c}_{p\alpha} \hat{c}_{p\beta},
\]
where \( \hat{c}_{p\alpha} \) (\( \hat{c}_{p\alpha} \)) are creation (annihilation) operators.

From this expression and by use of Kubo’s formula we obtain the axial Hall conductivities,
\[
\tilde{\sigma}_{zr}^{\text{DC}}(T) = -\frac{1}{V} \sum_{p, \alpha} f(\epsilon_{p}^\alpha) B_{zr}^{\alpha}(p),
\]
\[
\tilde{\sigma}_{xz}^{\text{DC}}(T) = -\frac{1}{V} \sum_{p, \alpha} f(\epsilon_{p}^\alpha)p_{0} \cos \varphi B_{xz}^{\alpha}(p),
\]
where \( B_{\mu\nu}^{\alpha}(p) = -2i \text{Im} \langle \partial_{p_{\mu}} u_{\alpha}(p) | \partial_{p_{\nu}} u_{\alpha}(p) \rangle \) is the Berry curvature, which is given by
\[
B_{zr}^{\pm}(p) = \mp \frac{\Delta v_{F}}{2(v_{F}^{2}q_{r}^{2} + \lambda^{2}p_{z}^{2} + \Delta^{2})^{3/2}},
\]
\[
B_{xz}^{\pm}(p) = \pm \frac{\Delta v_{F} \cos \varphi}{2(v_{F}^{2}q_{r}^{2} + \lambda^{2}p_{z}^{2} + \Delta^{2})^{3/2}}.
\]