Dynamical Piezoelectric and Magnetopiezoelectric Effects in Polar Metals from Berry Phases and Orbital Moments

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The polarization of a material and its response to applied electric and magnetic fields are key solid-state properties with a long history in insulators, although a satisfactory theory required new concepts such as Berry-phase gauge fields. In metals, quantities such as static polarization and the magnetoelectric $\theta$ term cease to be well defined. In polar metals, there can be analogous dynamical current responses, which we study in a common theoretical framework. We find that current responses to dynamical strain in polar metals depend on both the first and second Chern forms, related to polarization and magnetoelectricity in insulators as well as the orbital magnetization on the Fermi surface. We provide realistic estimates that predict that the latter contribution will dominate, and we investigate the feasibility of experimental detection of this effect.

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Introduction.—The importance of Berry phases and other geometrical properties of Bloch wave functions was first clearly understood in topological phases such as the integer quantum Hall effect [1,2]. It rapidly became clear that many physical observables in solids are described by Berry phases even in ordinary insulators with no quantization; the electrical polarization in a crystal can be fully and concisely expressed via the Berry connection of Bloch states [3,4]. Metallic systems present additional challenges: in the oldest example, the anomalous Hall effect [5], there are both Berry curvature “intrinsic” contributions and “extrinsic” contributions that depend on the details of scattering processes. Discrete symmetries underlie and restrict the emergence of these responses [6]; the anomalous Hall effect is enabled by the breaking of time-reversal symmetry and is observed in magnetic metals.

The goal of this Letter is to analyze a class of transport effects enabled by the breaking of inversion symmetry in metals. The study of inversion breaking materials such as ferroelectric insulators with switchable polarization, has revealed several fundamental pieces of solid-state physics and led to a variety of applications [7,8]. These advances have translated into a recent increasing interest in the more elusive polar metals [9–11]. While metals do not have a measurable electrical polarization—any surface charge density would be screened by the bulk conduction electrons—polar metals have a low enough symmetry group to support a static polarization were they insulators. More precisely, we explain how the Berry curvature and related quantities such as the orbital magnetic moments [12] result in a piezoelectric and magnetopiezoelectric (MPE) response to time-dependent strain in polar metals with or without time-reversal symmetry. Some of these observables can be viewed as generalizations to metals of Berry curvature properties in insulators such as electrical polarization and the orbital magnetoelectric effect, while others are Fermi Surface (FS) properties and, hence, specific to metals. The effects we discuss have important analogues in the corresponding insulating inversion-broken state, in the same way as the integer quantum Hall effect is connected to the intrinsic anomalous Hall effect [13,14]. An additional motivation for the present Letter is the active theoretical discussion of when metals, such as Weyl semimetals [15,16], can support a current that is induced by and is parallel to an applied magnetic field (the chiral magnetic effect) [17–24]. The answer is connected to the low-frequency limit of optical activity and involves the magnetic moment of Bloch electrons at the Fermi level [25,26], which raises the question of what other properties of metals might involve such magnetic moments.

The main results of the present Letter are summarized in equations (12)–(15) and Table I compiles the symmetry requirements for the effects to emerge. The first is referred to as piezoelectricity [27–29]; in a polar material, even in a metal, any time-dependent change of the material, such as a time-dependent strain, will induce a current resulting from the change of polarization. In a metal, only changes in polarization are well-defined as these involve measurable bulk currents through the unit cell. As a difference with the insulating case where the energy gap protects against processes that do not excite electrons far from the ground state, we will require a slow evolution of strain relative to electronic time scales [30]. This assumption guarantees that the distribution function remains close to equilibrium. Additional effects from strongly nonequilibrium distributions and the scattering processes that restore equilibrium are left for future work.
A second effect, which we call magnetopiezoelectricity, emerges when the material is magnetically ordered and time-reversal symmetry is broken along with inversion symmetry. This second order current response is bilinear in strain rate and static external magnetic field [Fig. 1(a)]. One contribution can be viewed as the generalization to metals of the orbital magnetoelectric effect in insulators [32–35]. It involves the second Chern form of the Berry gauge fields [36–38], a slightly more complicated geometrical object than the first Chern form that controls the polarization and Hall effect, and can be interpreted as a metallic version of the dynamical axion effect in antiferromagnets [39,40].

We also find a second, purely Fermi-surface contribution to the MPE that is proportional to the orbital magnetic moment. Our estimates for realistic systems suggest that this part of the MPE, unique to metals, dominates the response. Therefore, it is the main prediction of this Letter for a new experimental effect.

Methodology.—To address the topological responses of metallic magnetoelectrics, we employ a semiclassical formalism [12,13,36,41–43]. Our starting point is a three-dimensional Hamiltonian of a metal \( H(\mathbf{k}, \theta) \) that is parametrized by a time-dependent parameter \( \theta(t) \). The microscopic origin of \( \theta(t) \) can be diverse, it can, for example, parametrize ferromagnetic [44] or antiferromagnetic ordering [45]. Such a fluctuating magnetic order in insulating systems has been previously studied [46] and termed “dynamical axion field.”

In this Letter, we focus on the case where \( \theta \) emerges from the coupling of homogeneous time-dependent strain to orbital degrees of freedom, which effectively renormalizes the hopping structure of \( H(\mathbf{k}) \) in a time-dependent fashion leading to \( H(\mathbf{k}, \theta) \). The parameter \( \theta \) can refer to any strain component, or an arbitrary parametrization of some combination of strain components. Before proceeding, it is worth highlighting several relevant aspects of our calculation. First, strain is nonelectromagnetic and acts as an independent external field. Second, although we allow for the time-reversal-breaking magnetic order required for the MPE to depend on \( \theta \), we assume it does not respond to external magnetic fields at the linear order of interest here. Thus, we only focus on the orbital contribution. Finally, we assume the clamped ion limit; strain changes the hopping amplitudes for the electrons, but the atomic coordinates remain fixed.

A compact way of dealing with \( H(\mathbf{k}, \theta) \) is to regard \( \theta \) as an extra momentum coordinate. The semiclassical equations governing the dynamics in this case are given by

\[
\dot{\mathbf{r}}^i = \frac{1}{\hbar} \frac{\partial \tilde{\mathcal{E}}_{\mathbf{k}\theta}}{\partial \mathbf{k}^i} - (\tilde{\Omega} \times \tilde{\mathbf{k}})^j - \tilde{\Omega}^{ij} \mathbf{\dot{\theta}},
\]

\[
\hbar \mathbf{\dot{\theta}} = -eE_i - e(\mathbf{B} \times \mathbf{\dot{r}}),
\]

in terms of the external magnetic (\( \mathbf{B} \)) and electric (\( \mathbf{E} \)) fields, the \( i = x, y, z \) component of the three-dimensional position (\( \mathbf{r} \)) and momentum (\( \mathbf{k} \)). The Berry curvature components \( \Omega \) and \( \Omega^{ij} \) to be defined precisely below, determine the Hall conductivity [3] and the piezoelectric effect [29], respectively. For what follows, we find it convenient to promote the semiclassical picture to a four-dimensional space defined by an extended momentum and position vector [see Fig. 1(b)], \( \mathbf{k}_{\mu} = (\mathbf{k}, \theta) \) and \( \mathbf{r}_{\mu} = (\mathbf{r}, r_{\theta}) \), respectively, with \( \mu = x, y, z, \theta \) [47]. The semiclassical equations for such a phase space read [12,48]

\[
\dot{\mathbf{r}}^\mu = \frac{1}{\hbar} \frac{\partial \tilde{\mathcal{E}}_{\mathbf{k}\theta}}{\partial \mathbf{k}^\mu} - \tilde{\mathcal{E}}^{\mu \nu} \mathbf{\dot{\theta}},
\]

\[
\hbar \mathbf{\dot{\theta}} = -eE_\mu - eB_{\mu \nu} \mathbf{\dot{r}}^\nu.
\]

Here, \( E_\mu \) and the antisymmetric tensor \( B_{\mu \nu} \) are the generalization of the electric (\( E_i \)) and magnetic (\( B_i = \frac{1}{2} \epsilon_{ijk} B_{jk} \)) fields where by construction \( B_{\theta \theta} = 0 \) that implies, from (4), that \( \hbar \mathbf{\dot{\theta}} = -eE_\theta \). We note that Eq. (3) includes two corrections due to the external fields [12,49]. One modifies the band structure \( \epsilon_{\mathbf{k}, \theta} \rightarrow \tilde{\epsilon}_{\mathbf{k}, \theta} = \epsilon_{\mathbf{k}, \theta} - m_{\mathbf{k}, \theta} \cdot \mathbf{B} \) where \( m_{\mathbf{k}, \theta} = (e/2\hbar) \text{Im} (\partial_{\mathbf{k} \theta} u_{\mathbf{k}, \theta}) \times (H - H_{\mathbf{k}, \theta}) (\partial_{\mathbf{k} \theta} u_{\mathbf{k}, \theta}) \) is the magnetic orbital moment defined through the Bloch wave functions \( |u_{\mathbf{k}, \theta}\rangle \). Second, the unperturbed Berry curvature \( \Omega^{\gamma \rho} = \partial_{\mathbf{k} \rho} a_{\mathbf{k} \gamma} - \partial_{\mathbf{k} \gamma} a_{\mathbf{k} \rho} \) where \( a_{\mathbf{k} \gamma} = i \langle u_{\mathbf{k}, \theta} | \partial_{\mathbf{k} \theta} | u_{\mathbf{k}, \theta} \rangle \) is corrected as \( \Omega^{\gamma \rho} \rightarrow \tilde{\Omega}^{\gamma \rho} = \Omega^{\gamma \rho} + \Omega^{\gamma \rho}_{\mathbf{k}} (\tilde{\Omega}_{\theta} = \frac{1}{2} \epsilon_{ijk} \tilde{\mathcal{E}}^{ij} \tilde{\mathcal{E}}^{k}) \). The additional
\[ \Omega_{ij} = \partial_{k} d'_{ij} - \partial_{k} d_{ij}, \]
\[ \text{is defined by } d'_{ij} = i \langle u_{k,\theta} | \partial_{k} | u_{k,\theta} \rangle + \text{c.c.} \]
that incorporates the first-order correction to the Bloch wave function \(| u_{k,\theta} \rangle \). The quantity \( d'_{ij} \) is gauge invariant and physically corresponds to a shift of the wave-packet center induced by interband mixing from the external fields [49].

Combining (3) and (4) and keeping terms to second order in the external fields results in [48]

\[ j^{\mu} = e \int \frac{d^{3}k}{(2\pi)^{3}} D_{k,\theta} f(\tilde{\epsilon}_{k,\theta}, \mu). \]  

Here, \( f(\tilde{\epsilon}_{k,\theta}, \mu) \) is the Fermi-Dirac distribution for the perturbed band structure \( \tilde{\epsilon}_{k,\theta} \) at chemical potential \( \mu \) and \( D_{k,\theta} \) is the modified density of states defined as

\[ D_{k,\theta} = \left[ 1 + \frac{1}{2} \xi B_{\mu\nu} \tilde{\Omega}^{\mu\nu} + \mathcal{O}(B^{2}) \right]. \]

Using (5) and (6), the current density reads

\[ j^{\mu} = e \int \frac{d^{3}k}{(2\pi)^{3}} \left[ \frac{1}{\hbar} \frac{\partial \tilde{\epsilon}_{k,\theta}}{\partial \mu} E_{\nu} + \frac{e}{\hbar} \tilde{\Omega}^{\mu\nu} E_{\nu} \right] \]
\[ + \frac{e^{2}}{\hbar^{2}} \left( \tilde{\Omega}^{\mu\nu} B_{\nu} \tilde{\Omega}^{\rho\delta} \tilde{\Omega}^{\sigma\delta} \tilde{\epsilon} \right) \frac{\partial \tilde{\epsilon}_{k,\theta}}{\partial \mu} \]
\[ + \cdots. \]  

We are interested in the spatial components of current density \( j^{i} \) generated when \( E = 0 \). Keeping terms potentially linear in \( B \) results in [50]

\[ j^{i} = e \int \frac{d^{3}k}{(2\pi)^{3}} \left[ \frac{1}{\hbar} \frac{\partial \tilde{\epsilon}_{k,\theta}}{\partial \mu} \right] \frac{e}{\hbar} \tilde{\Omega}^{\mu\nu} B_{\nu} \]
\[ + \frac{e}{\hbar^{2}} \left( \tilde{\Omega}^{\mu\nu} B_{\nu} \tilde{\Omega}^{\rho\delta} \tilde{\Omega}^{\sigma\delta} \tilde{\epsilon} \right) \frac{\partial \tilde{\epsilon}_{k,\theta}}{\partial \mu} f(\tilde{\epsilon}_{k,\theta}, \mu) \]
\[ + \cdots. \]  

which is of the form \( j^{i} = j_{b}^{i} + j_{c}^{i} + j_{e}^{i} \). The last term, \( j_{c}^{i} \), can be proven to be zero [51] which is consistent with the absence of the chiral magnetic effect in the static limit [25,26]. In the second term, \( j_{b}^{i} \), keeping only linear order corrections in \( B_{i} \) allows us to evaluate the distribution function at the unperturbed energy \( \epsilon_{k,\theta} \) leading to

\[ j_{b}^{i} = - \frac{e^{2}}{8 \hbar} \int \frac{d^{3}k}{(2\pi)^{3}} \left[ (\epsilon_{\mu\nu\rho\sigma} \Omega^{\mu\nu} \Omega^{\rho\sigma}) \tilde{\epsilon} \right] f(\epsilon_{k,\theta}, \mu) B_{i}. \]
magnetoelastic effect in our semiclassical treatment, which neglects terms resulting from cross-gap contributions, which vanish as 1/Δ [34]. Second, the current generated by finite deformations is well defined since it is the integral of the second Chern form. The Chern-Simons three form is only gauge invariant if integrated over a closed manifold, so it does not correspond to a measurable quantity in metals; the static polarization is ill defined in metals.

Finally, the third term, α₃, is a novel Fermi surface contribution that is unique to metals. It is the correction to the piezoelectric response at linear order in the magnetic field due to the orbital moment of the Bloch states. In what follows, we estimate the magnitude of all three terms contributing to the current to find that the Fermi surface contribution dominates the response.

Experimental feasibility.—An estimate of the observability of the current in Eq. (12) relies on the magnitude of the Berry curvature Ωμν, which is common to all its terms. We have distinguished two contributions to Ωμν of distinct physical origin: the purely spatial part Ωij and the mixed Ωij terms. The former defines the Hall conductivity σij = Cijε2/h in the (i, j) plane through the Chern number Cij = (1/2π) ∫ d²kΩij. Since Cij is of the order of unity [52] or higher [53,54], we expect Ωij ≥ (a²/2π) where we estimate the cross sectional area of the unit cell in the (i, j) plane using the lattice spacing a. To estimate Ωij, we use previously known facts about the piezoelectric effect. Identifying θ with a specific strain component εijk (θ = εjk), the piezoelectric constant reads [29]

\[ P^i = \frac{\partial P^i}{\partial \theta^{jk}} = -e \int_{\text{occ}} \frac{d^5 k}{(2\pi)^3} \Omega^{ij}. \tag{16} \]

This formula only contains the electronic (clamped ion) contribution to the polarization response, typically smaller than the dominant contribution from the rearrangement of the ions. The electronic contribution can, nonetheless, be accessed independently in ab initio calculations that estimate \( \beta' \approx 1 \text{ C/m}^2 [55] \) (suppressing the strain component indices for clarity). It follows that \( \Omega^{ij} \sim \beta'(a^2/e) \) using the inverse cube of the lattice spacing as an approximate volume of the Fermi sea.

From the above estimate of the piezoelectric effect, we can now approximate the magnitude of the remaining terms in Eq. (12), \( \alpha_1 \) and \( \alpha_3 \), given by Eqs. (14) and (15), respectively, that are novel to this Letter. The magnitude of the Fermi sea contribution \( \alpha_1 \) amounts to

\[ \alpha_1 \sim \frac{e}{\hbar} a^2 C_{ij} \beta^k, \tag{17} \]

for a particular set of \( i \neq j \neq k \) and neglecting the order one factor arising from the difference between a Fermi sea integral and a Brillouin zone integral. Inserting \( \beta^k \sim 1 \text{ C/m}^2, \ a \sim 10^{-10} \text{ m}, C_{ij} = 1 \), we get \( \alpha_1 \sim 10^{-5} \text{ (A s/T m}^2). \)

The estimate of the magnitude of the Fermi surface term \( \alpha_3 \), unique to metals, requires the magnitude of the orbital magnetic moment \( |\mathbf{m}| \). A conservative estimate results in \( |\mathbf{m}| \sim \mu_B \sim 10^{-23} \text{ J/T} \) where \( \mu_B \) is the Bohr magneton, but it can be as large as \( |\mathbf{m}| \sim 30 \mu_B \) [12]. The area of the Fermi surface can be estimated as \( 1/a^2 \), the cross section of the BZ which is the inverse of the cross section of the real space unit cell. Taking \( v_F \sim 10^6 \text{ m/s} \), which is typical for metals but can be significantly smaller for lightly doped insulators near the band bottom, and using our above estimate for \( \Omega^{ij} \), we obtain

\[ \alpha_3 \sim \frac{\beta' m^2 a}{h v_F} \sim 10^{-4} \text{ A s/T m}^2. \tag{18} \]

Therefore, we conclude that \( \alpha_3 \geq \alpha_1 \), and the Fermi surface contribution specific to metallic systems is dominant.

In addition, it is relevant to emphasize the following important points regarding experimental detection. First, strain rates at the order of \( 10^{-2} \text{ s}^{-1} \) are achievable in the elastic regime using ultrasonic techniques [56,57]. For a sample at the cm scale, with cross sectional area \( A_s \sim 10^{-4} \text{ m}^2 \) and a magnetic field of \( 1 \text{ T} [58] \), the current signal is of the order of \( I_i = A_s j_i \sim 100 \text{ pA} \). Conventional ammeters have sensitivity extending to the pA range that is further improved in superconducting quantum interference devices.

Second, the magnetopiezoelectric effect is expected to coexist with the piezoelectric contribution, so accurate measurements over a range of magnetic fields are necessary for its detection. In our estimates, \( \alpha_2 \) is proportional to and much smaller than \( \beta \). However, \( \beta \) gets contributions from the entire Fermi sea, while \( \alpha_2 \) only depends on Fermi surface properties. This allows suppression of \( \beta \) without changing \( \alpha_2 \) in appropriately engineered band structures.

Third, the movement of the ions and the polarization of electrons in the valence bands induces a bound surface charge density. Part of the bulk current can be trapped screening it, possibly preventing its detection in our proposed setup (Fig. 1), but there is no reason to expect full cancellation. We note, as well, that pumping dc current is also possible by out-of-phase modulation of different strain components. Such a deformation path encircles a finite area in parameter space; the integral of the current for a pumping cycle is, in general, a nonvanishing, nonquantized value.

Finally, from the materials perspective, we find that MnSi satisfies most requirements for these effects to manifest. It is a magnetically ordered, inversion breaking metal with complex Berry curvature patterns in the conduction bands that is very susceptible to strain [59–62]. The magnetic order, however, is incommensurate and very sensitive to external magnetic field. An ideal candidate material would have a simple easy axis ferromagnetic or
Néel order that has vanishing susceptibility for magnetic fields in the ordering direction in the low temperature limit. The recently studied polar metals [10,11], while nonmagnetic, would provide a platform for realizing the field-independent piezoelectric response $\beta$. Cold-atomic systems also offer an alternative; the current is related to an field-independent piezoelectric response

$$\mathbf{v}_{\text{c.m.}} = \frac{\mathbf{j}}{n}$$

where $n$ is the density of the atomic cloud. Recently, $\mathbf{v}_{\text{c.m.}}$ has been exploited as a probe of topological properties [63] and it is, therefore, plausible that the effects we discuss here can be observed in these systems as well.

**Conclusion.**—We have calculated a novel magnetopiezoelectric response in inversion and time-reversal breaking metals subjected to static magnetic field and dynamic strain. Similar to the anomalous Hall effect in metals which can be viewed as a generalization of the quantized anomalous Hall effect in insulators, our results for magnetopiezoelectricity generalize the magnetoelectric response of insulators to metals. As a key difference, we find an additional Fermi surface contribution that relies on a finite orbital moment of metals. As a key difference, we find an additional Fermi surface contribution that relies on a finite orbital moment of electrons that is unique to metals and likely dominates the effect in real systems.

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