Recently, Kramers Weyl semimetals (KWS) with chiral lattice structures and Weyl points pinned at time-reversal invariant momenta have been discovered. However, the distinction between KWS and other Weyl semimetals in terms of physical properties is not clear. In this work, we show that KWS exhibit longitudinal magnetoelectric responses, which is the result of the specific form of spin-orbit couplings in KWS. The longitudinal magnetoelectric responses resemble the feature of classical solenoids in that the induced magnetization is parallel to the applied electric field. Importantly, in KWS with large effective mass and strong spin-orbit coupling, which is the case for several realistic materials, the induced magnetization can be two to three orders of magnitude larger than systems with the strongest Rashba spin-orbit couplings. We expect KWS to have important applications in nanoscale electromagnetic and charge-spin conversion devices.

Results

Effective Hamiltonians for Kramers Weyl Semimetals

In chiral crystals which respect time reversal symmetry, the energy bands are at least doubly degenerate at time-reversal invariant momenta due to the Kramers theorem. In the absence of inversion, mirror and improper rotation symmetries in chiral crystals, and away from the time-reversal invariant points, spin-orbit couplings would lift the Kramers degeneracy in momentum space to create

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ate Kramers Weyl points \[15\]. To be more specific, in the spin \(\frac{1}{2}\) basis \(\psi_k = [\phi_{k,\uparrow}, \phi_{k,\downarrow}]^T\), which satisfies the relation \(\Theta \psi_k = i\sigma_y \psi_{-k}\) under time-reversal operation \(\Theta = i\sigma_y K\), the effective Hamiltonian \(H_0(k)\) can be obtained through standard \(k \cdot p\) method \[15\]. Up to second order about a time-reversal invariant momentum \(k_0\), the general form of the Hamiltonian can be written as

\[
H_0(k) = \sum_{i,j} \frac{\hbar^2}{2m_{ij}} k_i k_j + \sigma_i \hbar v_{ij} k_j. 
\]  

(1)

Here, \(k\) is measured from \(k_0\), \(i,j = x,y,z\), \(m_{ij}\) is the effective mass tensor, \(v_{ij}\) are the Pauli matrices in spin space, and \(v_{ij}\) is the SOC pseudotensor. In chiral crystals, the small group at \(k_0\) is isomorphic to a chiral point group which guarantees \(\text{det}(v) \neq 0\) so that the Kramers Weyl point emerges at \(k = 0\). The specific forms of the SOC pseudotensor \(v_{ij}\) depend on the point group symmetry and the results are listed in the supplementary information \[20\] for all the chiral point groups.

For simplicity, we first start with materials with cubic point group symmetries \(\{T, O\}\) such as \(K_2\text{Sn}_2\text{O}_3\), \(\beta-\text{RhSi}, \text{CoSi}\), and \(\text{AlPt} \ [15,22]\). In these cases, for \(k_0\) with little group isomorphic to \(\{T, O\}\) at \(k_0\) (such as the \(\Gamma\) point), \(v_{ij}\) is proportional to the identity matrix and gives rise to an isotropic Weyl Hamiltonian with the form:

\[
H_0(k) = \frac{\hbar^2}{2m} k^2 + \hbar v k \cdot \sigma. 
\]  

(2)

The isotropic SOC \(v \cdot k \cdot \sigma\) creates a Weyl point at \(k_0\).

Another sample Hamiltonian that we are interested in describes Kramers Weyl points with chiral point group symmetry \(\{D_n\}\) with \(n = 2, 3, 4, 6\). Due to the lower crystal symmetry compared with the cubic groups, anisotropy shows up in the Weyl Hamiltonian as

\[
H_0(k) = \frac{\hbar^2}{2m_x} k_x^2 + \frac{\hbar^2}{2m_y} k_y^2 + \frac{\hbar^2}{2m_z} k_z^2 + \hbar v_x k_x \sigma_x + \hbar v_y k_y \sigma_y + \hbar v_z k_z \sigma_z. 
\]  

(3)

This Hamiltonian is relevant for \(\beta-\text{Ag}_{2}\text{Se}\), and elemental Te which have been experimentally studied recently \[20,27\]. It also describes the Kramers Weyl points of a few other materials such as \(\text{CsCuBr}_3\), which are shown to possess Kramers Weyl points through band structure calculations \[15\]. In the following sections, we will study the magnetoelectric effect of systems described by the isotropic and the anisotropic Weyl Hamiltonians. The simple form of the isotropic model allows us to calculate the magnetoelectric response analytically while the anisotropic case will be studied numerically.

**Magnetoelectric pseudotensors and their symmetry properties**

In magnetoelectric effects, induced magnetization \(M\) and the applied electric field \(E\) are related by the magnetoelectric pseudotensor \(\alpha\) such that:

\[
M_i = \sum_{i,j} \alpha_{ij} E_j, 
\]  

(4)

where \(i,j = x,y,z\) and \(\alpha_{ij}\) are elements of the the magnetoelectric pseudotensor \(\alpha\). For a generic Hamiltonian

\[
\mathcal{H} = \sum_{\nu,\nu'} c_{\nu,k}^\dagger H_{\nu,\nu'}(k) c_{\nu',k},
\]  

(5)

where \(c_{\nu,k}^\dagger\) \((c_{\nu,k})\) is the creation (annihilation) operator, \(H_{\nu,\nu'}(k)\) is the element of the Hamiltonian matrix \(H_0(k)\), \(\alpha_{ij}\) can be obtained from the linear response theory as \[24,25\]

\[
\alpha_{ij} = -\tau \frac{e}{\hbar} \left(\frac{1}{2\pi} \int d\mathbf{k} \sum_{n} M_{nk,i} \langle \psi_{nk}(\mathbf{k}) | \frac{\partial}{\partial \mathbf{k}} | \psi_{nk}(\mathbf{k}) \rangle \right) \frac{d\mathcal{E}(\mathbf{k})}{d\mathcal{E}_{nk}}.
\]  

(6)

In Eq.6 \(\mathcal{E}(\mathbf{k})\) is the Fermi Dirac distribution function, \(\mathcal{E}_{nk}\) is the energy dispersion of band \(n\) from the Hamiltonian \(H_0(k)\), \(v_{nk,j} = \frac{\partial E_{nk}}{\partial k_j}\), \(d\) is the dimension of the system, \(\tau\) is the effective scattering time and \(i,j = x,y,z\) denote the spatial components. The total magnetic dipole moment \(M_{nk} = \mathbf{S}_{nk} + \mathbf{m}_{nk}\) carried by the Bloch electrons consists of both the spin magnetic dipole moment \(\mathbf{S}_{nk} = \langle \phi_{nk} | \frac{1}{2} \sigma | \phi_{nk} \rangle\) and the orbital magnetic dipole moment \(\mathbf{m}_{nk} = \langle \phi_{nk} \big| \frac{\hbar}{\pi} (\partial k \phi_{nk}) \times [\mathbf{H}_0(\mathbf{k}) - \mathcal{E}_{nk}] \partial k \phi_{nk} \rangle\). Here, \(\mu_\text{s} = \frac{\hbar}{2 m} \) is the Bohr magneton, \(g\) is the Lande \(g\) factor which is set to be 2 in our calculations and \(\langle \phi_{nk} \rangle\) denotes a Bloch state. As we will show explicitly below, the orbital magnetization is related to the Berry curvature of the Bloch states which has the form \(\Omega_{nk} = i \langle \partial k \phi_{nk} \rangle \times [\partial k \phi_{nk} \rangle\). \[21\].

The linear response theory applies to generic Hamiltonians. However, to shed light on the general properties of KWS, we note that the form of \(\alpha\) can be determined by point group symmetries which is independent of the details of the Hamiltonian. The group theory analysis of \(\alpha\) is elaborated in the Methods section as well as in Ref. [36], and the general form for the chiral point groups is provided in Table I. From the group theoretical point of view, KWS can be classified into three sub-clases. For KWS belonging to the cubic \(\{T, O\}\) point groups, \(\alpha\) is proportional to the identity matrix as shown in Table I. This implies that the induced magnetization is always parallel to the direction of the applied electric field. Therefore, these KWS can behave as classical solenoids in all electric field directions without the need to fabricate any spiral structures.

For KWS with point groups \(D_n\), a pure longitudinal magnetisation parallel to the electric field is also obtained when the electric field is applied along the direction of any of the symmetry axes. For KWS with cyclic point groups, in general, magnetization with components parallel and perpendicular to the direction of the applied electric field are generated. Interestingly, for all other Weyl semimetals without chiral point group symmetry,
TABLE I: List of Magnetoelectric susceptibility pseudotensor $\alpha$ for the chiral crystals in the 11 chiral point groups. $\alpha_{ij}$ with $i, j = x, y, z$ are in general the elements in $\alpha$. $\alpha_{ij,\perp}$ represent the diagonal elements $\alpha_{xx,yy}$ and $\alpha_{zz}$ respectively. The $\alpha_{0}$ are the anti-symmetric elements and $\alpha_{0}$ represents the identical diagonal element in T and O group.

| Point group | $\alpha$ | Point group | $\alpha$ |
|-------------|----------|-------------|----------|
| O           | \[
\begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\] | T          | \[
\begin{pmatrix}
0 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & 0
\end{pmatrix}
\] |
| D$_2$       | \[
\begin{pmatrix}
\alpha_{xx} & 0 & 0 \\
0 & \alpha_{yy} & 0 \\
0 & 0 & \alpha_{zz}
\end{pmatrix}
\] | D$_3$      | \[
\begin{pmatrix}
\alpha_{xx} & 0 & 0 \\
0 & \alpha_{yy} & 0 \\
0 & 0 & \alpha_{zz}
\end{pmatrix}
\] |
| D$_4$       | \[
\begin{pmatrix}
0 & \alpha_{xx} & 0 \\
\alpha_{xx} & 0 & 0 \\
0 & 0 & \alpha_{zz}
\end{pmatrix}
\] | D$_6$      | \[
\begin{pmatrix}
0 & \alpha_{xx} & 0 \\
\alpha_{xx} & 0 & 0 \\
0 & 0 & \alpha_{zz}
\end{pmatrix}
\] |
| C$_1$       | \[
\begin{pmatrix}
\alpha_{x} & -\alpha_{y} & 0 \\
-\alpha_{x} & \alpha_{y} & 0 \\
0 & 0 & \alpha_{z}
\end{pmatrix}
\] | C$_2$      | \[
\begin{pmatrix}
\alpha_{x} & -\alpha_{y} & 0 \\
-\alpha_{x} & \alpha_{y} & 0 \\
0 & 0 & \alpha_{z}
\end{pmatrix}
\] |
| C$_3$       | \[
\begin{pmatrix}
0 & 0 & \alpha_{x} \\
0 & 0 & \alpha_{y} \\
\alpha_{x} & \alpha_{y} & 0
\end{pmatrix}
\] | C$_4$      | \[
\begin{pmatrix}
0 & 0 & \alpha_{x} \\
0 & 0 & \alpha_{y} \\
\alpha_{x} & \alpha_{y} & 0
\end{pmatrix}
\] |
| C$_6$       | \[
\begin{pmatrix}
\alpha_{x} & -\alpha_{y} & 0 \\
-\alpha_{x} & \alpha_{y} & 0 \\
0 & 0 & \alpha_{z}
\end{pmatrix}
\] | C$_5$      | \[
\begin{pmatrix}
\alpha_{x} & -\alpha_{y} & 0 \\
-\alpha_{x} & \alpha_{y} & 0 \\
0 & 0 & \alpha_{z}
\end{pmatrix}
\] |

the magnetoelectric response is zero if the electric field is applied along the principal axis [30]. Therefore, the longitudinal magnetoelectric response along the principal symmetry axis is a very distinctive feature of KWS due to the special spin texture of KWS which determines the spin and orbital magnetization.

In the following sections, we calculate $\alpha_{ij}$ explicitly using the isotropic and the anisotropic Weyl Hamiltonians given in Eq.[2] and Eq.[3] respectively. We demonstrate that, for certain KWS, the magnetoelectric response is two to three orders of magnitude larger than systems with the largest Rashba spin-orbit couplings.

**Longitudinal Magnetoelectric Response in Isotropic KWS**

We first consider an effective Hamiltonian which describes a Kramer Weyl point near the $\Gamma$ point in chiral crystals with point groups $\{T, O\}$ where the isotropic Weyl Hamiltonian is $H_0(k) = \frac{k^2}{2m}k^2 + \hbar c \mathbf{k} \cdot \sigma$. At Fermi energy $E_F = \frac{k_F^2}{2m}k^2 \pm \hbar v_k|\mathbf{k}|$, there are two spherical Fermi surfaces with corresponding wave vectors $\mathbf{k}_F \pm = \frac{\pm \sqrt{2mE_F + m^2v^2 + m^4}}{\hbar}$. The spin and orbital magnetic dipole moments of the two Fermi surfaces with Fermi momenta $\mathbf{k}_F \pm$ can be written as:

$$S_{k_F \pm} = \pm \frac{g_e \hbar}{2m_e} \mathbf{k}_F \pm, \quad m_{k_F \pm} = \frac{ev}{2} \frac{\mathbf{k}_F \pm}{|\mathbf{k}_F \pm|}. \quad (7)$$

It is important to note that the orbital magnetic moment $m_{k_F \pm}$ is proportional to the Berry curvature generated by the Weyl point on the Fermi surfaces which is $K_{F \pm} = \mp |\mathbf{k}_F \pm| \mathbf{e}$. The spin texture on a Fermi surface is schematically shown in Fig.[1](a). It is clear that without breaking time-reversal, the total magnetic moment of all the electrons is zero. By applying an electric field, the steady state distribution of the electronic state can generate a net magnetization as indicated in Eq.[6]. With this special form of spin texture of an isotropic KWS, at the Fermi energy $E_F$, we obtain the isotropic longitudinal magnetoelectric susceptibility $\alpha_0$ as:

$$\alpha_0 = \frac{e^2 v k}{\hbar^2} \sqrt{2mE_F + m^2v^2} \left( \frac{m}{m_e} - 1 \right). \quad (8)$$

In $\alpha_0$, the first and second terms are the spin and the orbital contributions respectively. From Table I, the magnetoelectric response of an isotropic KWS can be written as $M = \alpha_0 E$ which indicates that the magnetization induced is parallel to the applied electric field as is schematically shown in Fig.[1](b). From Eq.[8], it is clear that a large magnetoelectric response will be obtained with strong Weyl SOC $v$, long scattering time $\tau$, and a large effective mass $m$.

To seek a large magnetoelectric response from realistic materials, we note that, for example, the Weyl points of $K_2Sn_2O_3$ belonging to the cubic group $T$ have large effective mass for some Kramers Weyl points and strong spin-orbit couplings [33]. To estimate $\alpha_0$ for these cases, we set the isotropic Weyl SOC strength to be $\hbar v = 10$meV$\cdot$nm, effective mass $m = 20m_e$ where $m_e$ is the electron mass, and the electron scattering time $\tau = 6ps$. Then, $\alpha_0$ as a function of Fermi energy $E_F$ is calculated. The results are shown in Fig.[1]. It is important to emphasis that Kramers Weyl points are pinned at time-reversal invariant momenta. Therefore, electrons on opposite sides of the Weyl point have opposite spin. As a result, the spin-orbit coupling suppresses elastic backscattering from scalar impurities, similar to the case in the surface states of topological insulators [32–34]. The Weyl SOC enhanced scattering time is demonstrated in the Supplementary Materials [33] using Born approximation. Therefore, we choose a scattering time at 6ps which equals to the inter Weyl point scattering time in TaAs [35]. For Weyl points that appear at arbitrary momenta, the spin-orbit coupling suppression on backscattering within a Weyl point is expected to be weak due to a more uniform spin texture. This is another distinction between KWS and other Weyl semimetals.

It is important to note that the Kramers Weyl points can be located at other time-reversal invariant momenta. Take a N point of $K_2Sb_2O_3$ as an example, the effective Hamiltonian is not described by an isotropic Hamiltonian as the little groups are different between the N point and the $\Gamma$ point. However, by summing the contribution of all the 6 N points, and isotropic magnetoelectric response is recovered as dictated by the crystal symmetry. However,
My Mz a b Ex Ey Ez Mx c d μ0α0 (Tm/V) ×10−7
-8 -4 0 4 8
k (nm−1)
0
20
40E (meV)
0 20 40 60
E F (meV)
0
0.5
1
FIG. 1: The longitudinal magnetoelectric response in the KWS. (a) The Weyl spin texture held by the isotropic Weyl SOC \( v k \cdot \sigma \) at the Fermi surface from the band branch +. (b) The electrically induced magnetization is parallel to the applied electric field. (c) The energy dispersion for the isotropic chiral Weyl semimetal. (d) The magnetoelectric susceptibility \( \alpha_0 \) strength as a function the Fermi energy \( E_F \). \( \mu_0 \) is the vacuum permeability.

due to the presence of the six non-equivalent N points, there is roughly a further six-fold enhancement in \( \alpha_0 \) for the magnetoelectric response. This can result in a strong magnetoelectric response. Assuming that the chemical potential is 20meV above the Weyl point, an electric field of \( 10^5 \) V/m is enough to generate a magnetic field of 450G. It is two to three orders of magnitude larger than the magnetoelectric response of Au(111) surfaces and Bi/Ag bilayers which have large Rashba spin-orbit couplings [28, 29]. In these cases, the same strength of electric field can generate a magnetic field of order 1 to 10 G in Au(111) surfaces and Bi/Ag bilayers respectively [29].

Anisotropic longitudinal magnetoelectric response in KWS in dihedral point groups

For KWS with dihedral point group symmetry, the effective Hamiltonian near the Weyl point can be described by Eq.3. There are materials with large effective mass and strong spin-orbit coupling. For example, CsCuBr₃ belongs to the D₂ point group. From a symmetry point of view, the effective Hamiltonian of CsCuBr₃ near a Weyl point at \( \mathcal{M} \) takes the form of Eq. 3. From Table I, only the diagonal elements of the magnetoelectric pseudotensor are non-zero. We set \( m_x = 26m_e, m_y = 30m_e, m_z = 18m_e, v_x = 11\text{meV-nm}, v_y = 15\text{meV-nm} \) and \( v_z = 10\text{meV-nm} \). The \( \alpha_{ii} \) are calculated. The result is further enhanced by a factor of three as there are three \( \mathcal{M} \) points in the material. The final results are shown in Fig. 2 where a large magnetoelectric response is demonstrated.

Discussion

We note that the current induced magnetization in Weyl semimetals was first studied by Johansson et al. in TaAs which belong to the point group \( C_{4v} \) with mirror planes [29]. Therefore, the Weyl points appear at general \( k \) points and the resulting spin polarization induced by an electric field is perpendicular to the direction of the electric field. This transverse magnetoelectric effect is similar to the case with Rashba spin-orbit coupling which is a property of the polar point group as shown in Supplementary Materials [23, 30]. If the applied electric field is along the principal axis, however, the magnetoelectric response is zero in TaAs as determined by the \( C_{4v} \) point group symmetry which is one of the polar point groups.

On the other hand, the longitudinal magnetoelectric response in Weyl semimetals was first studied by Yoda et al. [37, 38]. However, in their models, helical hopping textures [37, 38] are needed for electrons to hop in a spiral manner, imitating the movement of electrons in a solenoid. As a result, it is natural to expect that an orbital magnetization parallel to the direction of an applied electric field would be generated and the effect is present without spin-orbit coupling. Unfortunately, no realistic materials that possess such helical hopping textures were identified. In this work, the origin of the longitudinal response is purely induced by spin-orbit coupling of KWS and the form of the response is dictated by the point group symmetry of the crystal.

Concerning material realizations, Kramers Weyl points generally exist in chiral crystals with spin-orbit coupling.

FIG. 2: The anisotropic magnetoelectric susceptibility \( \{\alpha_{xx}, \alpha_{yy}, \alpha_{zz}\} \) as a function of the Fermi energy \( E_F \) for the KWS in dihedral point groups.
However, to have a strong magnetoelectric response, it is preferable to have Kramers Weyl points with large effective mass and strong spin-orbit coupling. Unfortunately, the Kramers Weyl points can be far away from the Fermi energy and doping would be needed to reach these Weyl points. Further exploration will be needed to identify materials with large effective mass and strong SOC for the practical applications of KWS in magnetoelectric and charge-spin conversion devices.

Methods

Symmetry Analysis for the Magnetoelectric Response in Chiral Crystals

In the chiral crystals with magnetoelectric effect $M_i = \sum_{i,j} \alpha_{ij} E_j$ with $i, j = x, y, z$, under the crystal symmetry the magnetization transforms as $M_i \rightarrow \hat{R} R_i M_j$ while the electric field transforms as $E_i \rightarrow \hat{R} R_i E_j$, where $\hat{R}$ represents the symmetry transformation operator and is an orthogonal matrix. As a result, the magnetoelectric susceptibility $\alpha_{ij}$ under the crystal symmetry respects

$$\alpha = \text{det}(\hat{R}) \hat{R} \alpha \hat{R}^T.$$  

(9)

The chiral point groups, which do not allow improper rotations, can be divided into three sub-classes: the cubic point groups $\{T, O\}$, the dihedral point groups $\{D_n\}$ with $n = 2, 3, 4, 6$ and the cyclic point groups $C_n$ with $n = 1, 2, 3, 4, 6$. In the cubic point groups $\{T, O\}$, the multiple high order rotation axes along different directions would force the magnetoelectric susceptibility to be proportional to the identical matrix. In the dihedral point groups $\{D_n\}$ with $n=2, 3, 4, 6$, the $C_n$ rotation axis along $z$ and the in-plane $C_2$ rotation axis along the $x$-axis would eliminate all the off diagonal elements and leave only the diagonal elements in the magnetoelectric susceptibility $\alpha = \text{diag}(\alpha_{xx}, \alpha_{yy}, \alpha_{zz})$. In $\{D_3, D_4, D_6\}$, the principal axis would further make $\alpha_{xx} = \alpha_{yy}$. In the cyclic point groups $\{C_n\}$ with $n = 1, 2, 3, 4, 6$, the lower symmetry would allow the off-diagonal elements to coexist with the diagonal elements. The explicit forms of the magnetoelectric susceptibility pseudotensor $\alpha_{ij}$ from the symmetry analysis is shown in Table I for the 11 chiral point groups. The general forms of $\alpha$ for all noncentrosymmetric point groups with nonvanishing $\alpha$ are given in the Supplementary Materials.

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