Nonsymmorphic Topological Quadrupole Insulator in Sonic Crystals

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We present a theory for the quantized topological quadrupole moment in a class of 2D nonsymmorphic crystals with two glide symmetries, using sonic crystals as concrete examples. Intriguingly, the topological quadrupole moment arises from the difference in two Wannier orbitals and is hence denoted as the relative quadrupole moment. The quantization of the quadrupole moment is proven from the symmetry constraints and is verified numerically by the (nested) Wannier bands and the generalized Resta’s theory. We elaborate on the unique properties of this relative quadrupole topological insulator through its band structure, edge and corner states, and topological transitions.

Introduction.—Topological insulators are unconventional materials which host robust edge states and quantized response as dictated by the topological invariants of the occupied bulk Bloch bands. These topological invariants result from nontrivial quantization of Berry’s phases arising from parallel transport in the Brillouin zone, which are also related to topological charge pumping and dipolar topological polarization. Though developed to describe electronic systems, topological band theory can also be extended to photonic, acoustic, and elastic waves where the energy bands realize RQTI in the gray band gap. (a) Acoustic band structure for a = 2 cm. Red symbols ± label the parities at the Γ and X points. Right panel: unit-cell and the Brillouin zone of the sonic crystal with four arch-shaped scatterers made of epoxy. (c) The Wannier bands for the four acoustic bands below the gap (left), for the difference Wannier sector (middle), and for the same Wannier sector. (d) Nested Wannier bands for the Wannier bands and their difference below and above the polarization gap. l = 0.42a, h=0.21a, and w = 0.1a.

principle, can also be applied to other physical systems. The final outcome is an anomalous QTI with at least four bands below the topological gap, of which the four Wannier bands are non-degenerate and gapped. For the two Wannier bands below the polarization gap, we find that the topological quadrupole moment emerges from the difference between the two Wannier orbitals, whereas...
the sum of them gives a quantized dipole [see Fig. 1(a)], which cancels with another quantized dipole due to the other two Wannier bands above the polarization gap. This unprecedented topological phase, denoted as the relative quadrupole topological insulator (RQTI), is the focus of study in this Letter.

**Nonsymmorphic sonic crystals.**—The square-lattice sonic crystal is designed according to Fig. 1(a) with a lattice constant \(a\) (\(a \equiv 1\) unless specified). In each unit-cell, four arch-shaped blocks made of epoxy which serve as hard-wall scatterers for acoustic waves. The arch-shaped blocks are of identical geometry which is characterized by the width \(w\), the arch height \(h\), and the arch length \(l\). The four scatterers are arranged in a way that the sonic crystal has two orthogonal glide symmetries, \(G_x = \{m_x|\tau_y\}\) and \(G_y = \{m_y|\tau_x\}\) where \(m_x := x \rightarrow -x\), \(m_y := y \rightarrow -y\), \(\tau_y := y \rightarrow y + \frac{a}{2}\) and \(\tau_x := x \rightarrow x + \frac{a}{2}\) with \(a\) being the lattice constant. The structure is assumed to be two-dimensional (2D), while in experiments this can be realized by using epoxy boards cladding from both above and below to form a quasi-2D system [39]. In addition to the glide symmetries, the sonic crystal also has inversion \(P\) and the \(C_4\) rotation symmetries. These symmetries comprise a minimum set of nonsymmorphic crystalline symmetry that is needed for the quantized relative quadrupole moment.

The acoustic band structure is calculated using the commercial finite element solver, COMSOL Multiphysics. As shown in Fig. 1(b), there is a band gap between the fourth and the fifth acoustic bands which is the band gap of concern throughout this Letter. Under the inversion and \(C_4\) symmetries, the topological dipole polarization of acoustic bands can be determined by the parity eigenvalues at the high symmetry points [29].

\[
P_x = P_y = \frac{1}{4}(1 - \xi), \quad \xi = \Pi_n I_n(\Gamma)I_n(X), \quad (1)
\]

where \(n\) runs over all bands below the gap of interest, \(I_n(\Gamma)\) and \(I_n(X)\) give the parity eigenvalues for the \(\Gamma\) and \(X\) points, respectively. From the parity eigenvalues, one finds that the first two acoustic bands constitute a quantized topological dipole of \(\vec{P} = (\frac{\pi}{2}, \frac{\pi}{2})\). The same scenario applies to the third and fourth bands. Thus, the relative QTI needs at least four bands below the gap to ensure vanishing dipole polarization which is a necessary condition for the emergence of a quadrupole moment [28].

Effects of glide symmetries on the Bloch bands.— On the glide invariant lines such as the \(\Gamma X\) line for the \(G_y\) operator and the \(\Gamma Y\) line for the \(G_x\) operator, the Bloch states become the eigenstates of the glide operation. For instance, the first and second acoustic bands belong to the same eigenvalue of the \(G_y\) operator on the \(\Gamma X\) line, \(G_y \psi_{n,\vec{k}} = e^{i\frac{2\pi}{a}n} \psi_{n,\vec{k}}\) where \(n = 1, 2\) is the band index and \(\vec{k}\) is the wavevector. Along the \(\Gamma X\) line, the first band evolves into the second band after \(\frac{2\pi}{a}\) evolution of the glide operation. In this way, the \(\frac{2\pi}{a}\) periodicity of the glide eigenvalue is made to be compatible with the \(\frac{2\pi}{a}\) periodicity of the Brillouin zone [see Supplemental Materials]. In general, the glide operations, \(G_x\) and \(G_y\), connects two Bloch bands together. In our sonic crystal, the first and second bands form such a pair connected by the glide symmetry, while the third and fourth bands form another pair.

The glide symmetries also lead to double degeneracy for all Bloch states on the \(XM\) and \(YM\) lines. This double degeneracy can be understood by constructing the anti-unitary operators \(\Theta_j = G_j = T\) \((j = x, y)\) where \(T\) is the time-reversal operator (i.e., complex conjugation for acoustic Bloch wavefunctions). It is straightforward to obtain

\[
\Theta^2_y \psi_{n,\vec{k}} = e^{i\frac{2\pi}{a}n} \psi_{n,\vec{k}}. \quad (2)
\]

At the \(XM\) line where \(k_x = \frac{\pi}{a}\), one finds that \(\Theta^2_y \psi_{n,\vec{k}} = -\psi_{n,\vec{k}}\). Similar to the Kramers theorem for fermions, such a relation results in double degeneracy for all Bloch states on the \(XM\) line [13, 22]. According to the \(C_4\) rotation symmetry, the \(YM\) line also hosts double degeneracy for all Bloch states.

The parity operator \(P\) is also connected with the glide operators,

\[
P = \tau^2_y G_x G_y = \tau^2_x G_y G_x. \quad (3)
\]
The two glide operators do not commute with each other

$$G_x G_y \psi_{n,k} = e^{i(k_x - k_y) a} G_y G_x \psi_{n,k},$$

(4)

except when $k_x = k_y$. The non-commutivity of the two glide operators are essential for the realization of a non-trivial quadrupole moment. As proven in Ref. [29], commuting operators lead to gapless Wannier bands and thus cannot support the QTI phase.

The double degeneracy at the X (Y) point consists of two Bloch states of opposite parities, since $\Theta_y \mathcal{P} = -\mathcal{P} \Theta_y$. In contrast, the doublets at the M point comprises two Bloch states of the same parity because $[\Theta_x, \mathcal{P}] = [\Theta_y, \mathcal{P}] = 0$. For the $\Gamma$ point, the symmetry representation becomes equivalent to the $C_{4v}$ symmetry. Therefore, the double degeneracy occurs only for the $p_x$ and $p_y$ representations of the $C_{4v}$ group which have the same parity. The even parity bands, i.e., $s$ and $d_{xy}$ representations, are non-degenerate. In our sonic crystal, the $s$ and $d_{xy}$ representations are associated with the first and second bands, respectively. The the $p_x$ and $p_y$ representations are assigned to the third and fourth bands.

**Wannier bands and nested Wannier bands.**— One approach to verify the quantized topological quadrupole moment is to calculate the Wannier bands and nested Wannier bands. Using the acoustic Bloch wavefunctions from first-principle calculations, we obtained the Wannier bands using the Wilson-loop approach [43]. The results are presented in Fig. 1(c) where the Wannier centers $\nu_x$ for the four acoustic bands are calculated as functions of $k_y$. For each $k_y$, the Wilson-loop goes from $k_x = 0$ to $k_x = 2\pi/a$. The four Wannier bands are non-degenerate and separated by the polarization gap at $\nu_x = 0, \pm 0.5$. Note that each Wannier band has mixed contributions from all acoustic bands below the gap. For the region with $\nu_x \in (-0.5, 0)$, there are two Wannier bands. This feature, originating from the fact that we need four bands to cancel the dipole polarization (essentially due to the glide symmetries), is distinct from the conventional QTIs where there is only one Wannier band below the polarization gap.

We find that the symmetry constraints on the Wannier bands $\nu_{x,n}(k_y)$ are,

$$\nu_{x,n}(k_y) \equiv -\nu_{x,n'}(k_y) \mod 1,$$

(5a)

$$\nu_{x,n}(k_y) \equiv \nu_{x,n}(-k_y) \mod 1,$$

(5b)

$$\nu_{x,n}(k_y) \equiv -\nu_{x,n'}(-k_y) \mod 1,$$

(5c)

where $n'$ is often different from $n$. From Fig. 1(c) we find that the first (second) and fourth (third) Wannier bands have opposite polarizations. Because of the $C_4$ symmetry, the symmetry constraints on the Wannier bands $\nu_{y,n}(k_x)$ are similar to the above, which will not be studied in details here.

The two Wannier bands provide a larger space for topological phenomena. For instance, there can be two independent sectors. One is associated with the sum of the two Wannier bands, while the other is associated with the difference between the two Wannier bands. In principle, both Wannier sectors can have a nontrivial polarization and a quadrupole topological moment. However, our calculation indicates that the sum sector is trivial, whereas the difference sector gives a nontrivial quadrupole moment. In fact, the sum sector has gapless Wannier bands, since $\nu_{x,1}(k_x) + \nu_{x,2}(k_x) + \nu_{x,3}(k_x) + \nu_{x,4}(k_x) = 0.5 \mod 1$ give two quantized, canceling dipoles.

The quadrupole moment in the difference sector is verified first by the nested Wannier bands [4]. The nested Wannier bands quantify the topological edge polarization which is solely due to the quadrupole moment in 2D crystalline systems. Because there is no degeneracy in the Wannier bands, we can calculate the topological polarization for each Wannier band. The results are pre-
sented in Fig. 1(d) which indeed show that the difference Wannier sector gives a quantized topological edge polarization. The sum Wannier sector, in contrast, gives a non-quantized edge polarization.

The nested Wannier bands account for the topological edge polarization due to the quadrupole moment \(28, 29\). The topological edge polarization is given by

\[
p_{y}^{\nu} = \frac{1}{2\pi} \int dk_{x} p_{y}^{\nu,n}(k_{x}) \text{ mod } 1. \tag{6}
\]

Note that the above summation is taken within a particular Wannier sector. The nested Wannier band approach cannot determine which sector has a quantized quadrupole moment. Therefore, this method may miss the topological sector and obtain vanishing quadrupole moment for a quadrupole topological state \(37, 41\).

We find that the symmetry constraints only dictate that the Wannier band \(\nu_{x,n}\) has opposite edge polarization as that of the Wannier band \(-\nu_{x,n}\). For the topological edge polarization within a particular sector, a stronger restriction is obtained,

\[
p_{y}^{\nu_{x,+}} = -p_{y}^{\nu_{x,-}}, \quad p_{y}^{\nu_{x,+}} = 0, \quad \frac{1}{2} \text{ mod } 1. \tag{7a}
\]

\[
p_{y}^{\nu_{x,-}} = -p_{y}^{\nu_{x,+}}, \quad p_{y}^{\nu_{x,-}} = 0, \quad \frac{1}{2} \text{ mod } 1. \tag{7b}
\]

\[
p_{y}^{\nu_{x,0}} \equiv \sum_{n} \frac{1}{2\pi} \int dk_{x} p_{y}^{\nu_{x,n}}(k_{x}) \text{ mod } 1. \tag{7c}
\]

Therefore, the edge polarization for the Wannier bands below (denoted as “−”) and above (denoted as “+”) the polarization gap has to be quantized,

\[
q_{xy} = 2p_{y}^{\nu_{x,-}} p_{y}^{\nu_{x,-}} = \frac{1}{2}. \tag{9}
\]

Indeed, our calculation gives that our sonic crystal has \(p_{y}^{\nu_{x,-}} = -0.5\) and \(p_{y}^{\nu_{x,+}} = 0.5\) [see Fig. 1(c)]. According to the \(C_{4}\) symmetry, \(p_{y}^{\nu_{x,0}} = \frac{1}{2} p_{y}^{\nu_{x,+}} \). Therefore, there is a non-trivial quadrupole moment associated with the four acoustic bands,

\[
q_{xy} = 2p_{y}^{\nu_{x,-}} p_{y}^{\nu_{x,-}} = \frac{1}{2}. \tag{9}
\]

From the above we can see that an important feature of the nonsymmorphic QTI is that the edge polarization from each Wannier band is NOT quantized, although the symmetry constraints allow quantization of the edge polarization in certain sectors. These topological sectors turn out to be the difference Wannier sector, specifically, “1-2” for the region with \(\nu_{x} \in (-0.5, 0)\) and “4-3” for the region with \(\nu_{x} \in (0, 0.5)\).

Quadrupole topological index from generalized Resta’s approach.— To avoid the ambiguity in the nested Wannier band approach, we calculate the quadrupole topological number \(q_{xy}\) using the generalized Resta’s approach recently developed in Refs. \(40, 41\). This approach provides a rigorous quantum mechanical calculation of the quadrupole moment in crystals. The theory is developed for electronic systems without taking into account of spin degrees of freedom or the Coulomb interaction. Therefore, it can be directly translated to classical and bosonic systems. Specifically, the quadrupole topological number of a classical system is given by,

\[
q_{xy} = \frac{1}{2\pi} \text{Im}[\log \langle \tilde{U}_{\alpha} \rangle], \quad \tilde{U}_{\alpha} = \exp[2\pi i \sum_{r} Q_{xy}(\tilde{r})]. \tag{10}
\]

where the quadrupole operator is given by \(\hat{Q}_{xy}(\tilde{r}) = \frac{2\pi i L_{xy}}{L_{x} L_{y}} n(\tilde{r})\) with \(n(\tilde{r})\) being the probability density at the position \(\tilde{r}\). Here, we still use the quantum mechanical language, which will eventually be formulated using the acoustic Bloch wavefunctions. In the above equation, a finite system of size \(L_{x} \times L_{y}\), i.e., \(x \in [0, L_{x})\) and \(y \in [0, L_{y})\), with periodic boundary conditions is considered, yielding allowed wavevectors, \(\tilde{k} = (\frac{2\pi}{L_{x}}, \frac{2\pi}{L_{y}})\) with \(\alpha = 0, ..., L_{x} - 1\) and \(\beta = 0, ..., L_{y} - 1\). Taking into account of all Bloch states with the allowed wavevectors below the topological band gap, one finds that

\[
\langle \tilde{U}_{\alpha} \rangle = \text{det}(\hat{S}), \tag{11a}
\]

\[
S_{n,\tilde{k},m,\tilde{k}'} = \int d\tilde{r} \psi_{n,\tilde{k}}^{\ast}(\tilde{r}) \exp\left(\frac{2\pi i L_{xy}}{L_{x} L_{y}} \right) \psi_{m,\tilde{k}'}(\tilde{r}), \tag{11b}
\]

where the integral goes over the whole system. The above formulation is proven in Refs. \(40, 41\) to be a gauge-invariant and rigorous quantum mechanical definition of the quadrupole moment in crystals. Using this approach, our calculation shows that the quadrupole moment of our sonic crystal is precisely the nontrivial value \(q_{xy} = \frac{1}{2}\) (see Supplemental Materials).

FIG. 4. (Color online) Evolution of (a) edge states and (b) corner states during the process when the topological band gap closes (i.e., \(h \to 0\)). \(I = 0.42a\) and \(w = 0.1a\).
Topological edge and corner states.— The edge states induced by the topological quadrupole moment is calculated using a supercell structure which is periodic in the \( x \) direction but finite in the \( y \) direction. On one side of the supercell, we place a hard-wall boundary (HWB) condition with an air gap between the sonic crystal and the HWB [see the inset of Fig. 2(a)].

In a tight-binding model, the boundary is well-defined by the structure of the unit-cell. However, for sonic crystals and other physical systems where the band structure is induced by the multiple Bragg scattering mechanism, there is no such clear definition of boundaries, since the waves are propagating among the scatterers and are not obviously localized. Careful treatment of the boundary is often needed for topological sonic crystals. In fact, there is a subtle impedance matching issue at the boundary, as revealed in Ref. [44]. Our tuning of the air-gap is determined by two criteria: First, the emergence of topological edge states in the bulk band gap. Second, the corner states merge into the bulk bands precisely at the topological transition point. The first criterion is often easy to meet, whereas the second criterion can be satisfied only when the air-gap is equal to \( 0.28a \) for our sonic crystal. The second criterion excludes other mechanisms for the emergence of the corner states, since the corner states vanish when the topological quadrupole moment vanishes. Moreover, the width of the air-gap is sufficiently small, of which the corresponding cut-off frequency for the waveguide mode is 30 kHz for \( a = 2 \) cm. Therefore, the edge states are not mixed with the waveguide modes in the air-gap.

When a box-shaped super-structure with HWB is formed with both edges and corners [see inset of Fig. 2(c)], the system hosts the bulk, edge and corner states. By setting the air-gap to 0.28a, both the edge states and corner states are associated with the topological quadrupole moment. It is seen from Fig. 2(d) that there are indeed four degenerate corner states localized on the four corners of the sonic crystal. Remarkably, by using subwavelength sonic crystals, the quadrupole topological band gap in this Letter is very large, with a gap-to-midgap ratio of 49%. The resultant edge band gap is also large (21%). These very large band gaps lead to highly localized edge and corner states which are useful for subwavelength concentration of the acoustic fields.

Topological transitions.— As shown in Fig. 3(a), the emergence and disappearance of the quadrupole topology can be controlled by tuning the geometry of the sonic crystal. By reducing the arch height \( h \) for the scatterers, the quadrupole topological band gap can be made to close at \( h = 0 \). During this process, the edge and corner states, which are calculated using the same HWB as in Fig. 2, merge into the bulk. Importantly, since the corner states are solely induced by the bulk quadrupole moment, the corner states merge into the bulk bands only when the topological band gap is closed. In fact, our calculation shows that the corner states merge into the bulk bands at exactly the gap closing point with \( h = 0 \) [see Fig. 3(a)]. One can continue to tune the sonic crystal to reopen a trivial band gap where the sonic crystal has point group symmetry and vanishing quadrupole moment. Indeed, there is no corner states in the trivial band gap.

We calculate the evolution of the Wannier bands associated with the geometry-tuning process in Fig. 3(a). The results presented in Fig. 3(b) shows that the Wannier bands in the difference Wannier sector (“1-2” and “4-3”) are gapped in the topological region. They become gapless when the topological band gap is closed at \( h = 0 \) and remain to be gapless for the trivial band gap region. Fig. 3(c) shows that the quadrupole moment is nontrivial \( q_{xy} = \frac{1}{2} \) in the topological band gap region, whereas it is vanishing \( q_{xy} = 0 \) in the trivial band gap region. Here, the quadrupole moment \( q_{xy} \) is calculated using the generalized Resta’s approach.

The evolution of the wave functions of the edge states during the topological gap closing process is shown in Fig. 4(a). It is seen that the edge states gradually merge into the bulk, when the topological gap becomes smaller and smaller. As shown in Fig. 4(b), the corner states also merge into the bulk during the gap closing process. We also note from Fig. 3(a) that the edge gap remains finite during this process. The topological transition shown here is quite different from Ref. [45] where the corner modes merge into the edge (indicating that the corner states are induced by the topology of the edge states). These observations confirm that the corner and edge states originate from the nontrivial bulk topology, i.e., due to the topological quadrupole moment.

Conclusion and outlook.— Our study unveils a prototype QTI protected by orthogonal glide symmetries, which has distinctive features and properties from the conventional QTI. The same symmetry principle and mechanisms can, in principle, be realized in other physical systems such as photonic and plasmonic systems. Our study will trigger future works at the interdisciplinary field between subwavelength metamaterials and quadrupole topology which may have important applications as well.

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