Snowflake Topological Insulator for Sound Waves

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We show how the snowflake phononic crystal structure, which has been realized experimentally recently, can be turned into a topological insulator for sound waves. This idea, based purely on simple geometrical modifications, could be readily implemented on the nanoscale.

Introduction. – First examples of topologically protected sound wave transport have just emerged during the past three years. So far, experimental implementations exist on the centimeter-scale, both for the case of time-reversal symmetry broken by external driving [1], such as in coupled gyroscopes, as well as for the case without driving [2-5], such as in coupled pendula. Moreover, a multitude of different implementations have been envisioned theoretically [6-19]. However, it is highly desirable to come up with alternative design ideas that may be realized on the nanoscale, eventually pushing towards applications in integrated phononics. The first theoretical proposal in this direction [20] suggested to exploit the optomechanical interaction to imprint the optical vorticity of a suitably shaped laser beam to generate chiral sound wave transport in a phononic-photonic crystal. On the other hand, if one wants to avoid the strong driving by an external field, purely geometrical designs are called for. One remarkable idea of Mousavi et al. [21] posited creating a sound wave topological insulator by designing a phononic crystal structure made from a material that would be carefully engineered by a pattern of small holes to achieve degeneracy between vibrations that are symmetric and antisymmetric to the plane of the sample. The appearance of a fine-grained length-scale much smaller than the wavelength, however, makes it impossible to use this idea all the way down to wavelengths comparable to the smallest feature sizes allowed by nanofabrication. In the present manuscript, we propose a very simple modification to an already existing structure, the so-called snowflake phononic crystal. The snowflake crystal has already proven to be a reliable platform for nanoscale optomechanics [22], and could also support pseudomagnetic fields for sound waves [23]. With the proposed modification, which is inspired by an idea first analyzed by Wu and Hu for photonic systems [24] (see also [16, 17, 25]), one will be able to create a topological insulator for sound waves based on a proven nanoscale platform.

The envisaged system consists of snowflake-shaped holes of alternating sizes, in a periodic arrangement on a triangular lattice. This snowflake topological insulator can be viewed as a metamaterial that supports topologically protected sound waves whose typical wavelength is larger than the underlying lattice scale. Such elastic waves propagate along arbitrarily shaped domain walls engineered by appropriately varying the snowflake size. We will show that the topological protection is guaranteed if locally (at the lattice scale) the point group symmetry of the snowflake design is maintained.

Platform. – We assume a planar quasi-two-dimensional phononic crystal slab exhibiting a six-fold rotational symmetry ($C_6$) as well as a discrete translational symmetry ($T_a$) on a triangular lattice, with a lattice constant $a$. The most straightforward implementation consists in the snowflake phononic crystal. This crystal has been explored before in the context of optomechanics [22], since it is both a photonic and a phononic crystal, although we will only make use of its phononic properties. Its structure is shown in Fig. 1a.

Symmetries and folding. – Due to the $C_6$-symmetry, the acoustic band structure is forced to have Dirac cones at the two high-symmetry points, $\vec{K} = \pi/a(4/3,0)$ and $\vec{K}' = \pi/a(2/3,2/\sqrt{3})$. Now consider a single snowflake-shaped hole surrounded by six other such holes. Our aim will be to break the original translational symmetry by changing the central snowflake in this configuration, thereby enlarging the real-space unit cell by a factor of $\sqrt{3}$ (Fig. 1b). Conversely, this will reduce the size of the first Brillouin zone (BZ) by the same factor. To anticipate this reduction, we imagine what happens when the original band structure, obtained for the as-yet unperturbed structure, gets folded back into the new BZ (see Fig. 1b-b). This will map the Dirac cones from $\vec{K}$ and $\vec{K}'$ of the old BZ to the $\Gamma$-point of the new BZ, forming a degenerate pair of double Dirac cones at $\vec{K} = (0,0)$ (Fig. 1b).
Inversely with the linear dimensions, as usual).} \(\Delta r\) indicates the radius deviation of every third (red) snowflake. For the special case of \(\Delta r = 0\) we obtain a regular snowflake pattern with the discrete translational symmetry \(T_a\) (blue unit cell). (c) shows the corresponding band structure along a path passing the high symmetry points (blue BZ in b) that features Dirac cones at \(\tilde{K}\) and \(\tilde{K}'\). Describing the same system with an enlarged unit cell (red) results in a reduced BZ (red), folds the band structure, and maps both Dirac valleys to the Γ-point (d). \(\Delta r \neq 0\) breaks \(T_a\) but maintains \(T_{\tau}\) (requiring the red unit cell and red BZ) and \(C_6\). This gaps both Dirac double cones (e). In the band structures (c-e) modes symmetric to the x-y-plane are displayed in brighter colors. [Here we used \((a, r, w, d) = (5000, 1800, 750, 220)\) nm and assumed the crystal slab made of silicon (Si) with Young’s modulus of 170 GPa, mass density 2329 kg/m\(^3\), and Poisson’s ratio 0.28].

Only in the next step we actually do break \(T_a\), by carrying out the afore-mentioned change of the central snowflake, increasing the lattice constant \(a \rightarrow \tilde{a} = \sqrt{3}a\) and establishing the new symmetry \(T_{\tilde{a}}\), all the while preserving \(C_6\) around the unit-cell centers. This opens a complete gap at the Γ-point (Fig. 1b), which can be topological in nature, as will be explained below.

The easiest way to implement this modification of the geometry is to change the radius of the central snowflake in each (enlarged) unit cell by \(\Delta r\), with \(\Delta r = 0\) referring to the original snowflake crystal (Fig. 1a).

The band structures shown in Fig. 1 have been obtained from full finite-element simulations of the equations of linear elasticity, solving the eigenvalue problem

\[
\text{div} \left[ \mathbf{E} \left[ \text{grad} \psi + (\text{grad} \psi)^T \right] \right] = -2\varphi \omega^2 \psi, \\
\text{(1)}
\]

with \(\psi\) being the complex three-dimensional wave function related to the mechanical displacement field \(\mathbf{u} = \text{Re} \left[ \psi \cdot e^{i\omega t} \right]\) of the crystal, \(\mathbf{E}\) the elasticity tensor, and \(\varphi\) the mass density. Here \(\text{div}\) is a short-hand for the tensor product, \([\mathbf{E} : \text{grad} \psi]_{ij} = E_{ijkl} \partial_k \psi_l\). For concreteness, we envisioned a phononic crystal slab of thickness 220 nm, but much smaller slabs have been fabricated already, down to unit cells of only a few hundred nanometers lateral extension (acoustic frequencies would scale inversely with the linear dimensions, as usual).

Effective Hamiltonian. – We now derive an effective Hamiltonian valid for the vicinity of the Γ-point. We are taking a route that clarifies the connection to the original valley degree of freedom. The results can alternatively be understood in the framework of the symmetry arguments first advocated for \(C_6\)-symmetric structures in the photonic context in [24]. We start with the eigenstates of the two double Dirac cones of the regular \((\Delta r = 0)\) snowflake array. They are labeled by \(|\psi_{\sigma,\tau}\rangle\), with \(\sigma = \pm 1\) being the quasi-angular momentum with respect to the 3-fold rotation

\[
\hat{R}_{2\pi/3} |\psi_{\sigma,\tau}\rangle = e^{-i\sigma \frac{2\pi}{3}} |\psi_{\sigma,\tau}\rangle,
\text{(2)}
\]

and \(\tau\) denoting the valley degree of freedom \((\tau = +1\) for \(K\) vs. \(\tau = -1\) for \(K'\)). Under time reversal \(\hat{T}\) (complex conjugation) and inversion \(\hat{R}_\pi\) they obey

\[
|\psi_{\sigma,\tau}\rangle = \hat{T} |\psi_{-\sigma,-\tau}\rangle = \hat{R}_\pi |\psi_{\sigma,-\tau}\rangle.
\text{(3)}
\]

The exact mode shapes of \(|\psi_{\sigma,\tau}\rangle\) for the particular case of the original snowflake crystal are explained in detail in [23]. In order to derive the Hamiltonian, we use two sets of Pauli matrices to span the 4-dimensional Hilbert space. We define one set for the valley degree of freedom \(\hat{\tau}_{(x,y,z)}\) and another one for the quasi angular degree of freedom \(\hat{\sigma}_{(x,y,z)}\), such that \(\hat{\tau}_{z} |\psi_{\sigma,\tau}\rangle = \tau |\psi_{\sigma,\tau}\rangle\) and \(\hat{\sigma}_{z} |\psi_{\sigma,\tau}\rangle = \sigma |\psi_{\sigma,\tau}\rangle\), and the usual set of Pauli matrices holds in this basis.

We now write down the Hamiltonian as a Taylor series up to linear order in \(\tilde{k}\) by using the above matrices. We keep only terms that are invariant under \(\hat{T}\) and \(\hat{R}_{\pi/3}\), which are the symmetries of our snowflake crystal (even for \(\Delta r \neq 0\)). This leaves us with only the following terms:

\[
\hat{H}_k = g\hat{\tau}_x + v\hat{\tau}_z (k_x\hat{\sigma}_x + k_y\hat{\sigma}_y).
\text{(4)}
\]

Up to a unitary transformation this Hamiltonian is equivalent to the large-wavelength limit of the Bernevig-Hughes-Zhang model for a topological insulator [26]. The first term in Eq. (4) is induced by the breaking of the \(\hat{T}_a\) symmetry and is responsible for gapping the degenerate Dirac cones. In other words, \(g\) can be interpreted as a mass, which can change sign. The unitary symmetry that allows to cast Eq. (4) in a block-diagonal form is the spin degree of freedom \(\hat{S} = \hat{\sigma}_z\). Combined with the time-reversal operator, it gives rise to a pseudo time-reversal symmetry \((\hat{T}\hat{S})\), which has the peculiarity that it squares to minus the identity, directly leading to Kramer’s degeneracy. At the Γ-point, the common eigenstates of \(\hat{H}_{k=0}\) and \(\hat{S}\) are the states \(|p^+\rangle\) and \(|d^\pm\rangle\) which obey \(\tau_{x} |d^\pm\rangle = |d^\mp\rangle\), \(\tau_{z} |p^\pm\rangle = - |p^\mp\rangle\), \(\hat{S}|p^\pm\rangle = \pm |p^\pm\rangle\), and \(\hat{S}|d^\pm\rangle = \pm |d^\mp\rangle\). One can show that these states are actually of \(p^\pm\) and \(d^\pm\) type with respect to their behavior under 60-degree rotations:

\[
\hat{R}_{\pi/3} |p^\pm\rangle = e^{\pm i\pi/3} |p^\pm\rangle, \quad \hat{R}_{\pi/3} |d^\pm\rangle = e^{\pm i2\pi/3} |d^\pm\rangle.
\]

Note that away from the Γ point only states of the same helicity \((s = \pm 1)\) will get mixed to form the finite-\(k\)
Figure 2. Band inversion: Frequencies of the $|p^\pm\rangle$, $|d^\pm\rangle$ modes at the Γ-point $\vec{k} = 0$ evolving for a sweep of the central snowflake radius $r_c$. A snapshot of the corresponding displacement fields for $r_c = 1600$nm and $r_c = 2000$nm is also shown. The in-plane displacement field is directly visualized by the deformation, whereas the out-of-plane displacement is encoded in the colorscale. $d(p)$-orbitals are (anti-)symmetric under rotation by 180 degrees.

eigenstates. The Hamiltonian terms which are linear in the quasimomentum $\vec{k}$ will induce transitions only between states whose 60-degree quasi-angular momenta differ by one quantum: $p^+ \rightarrow d^+$ and $p^- \rightarrow d^-$. Only further away from the Γ-point, higher-order terms (e.g. $\sim k^2$) can eventually couple the $+$ and $-$ states, i.e. mix different helicities. An indirect signature of this coupling is the lifting of the degeneracy of the two helicities. Remarkably, for our specific design, the splitting remains smaller than 1.5% of the band gap even for a quasimomentum as large as 1/4 of the distance to the boundary of the Brillouin zone, $|\vec{k}| \leq \pi/(6a)$.

In a topological insulator, the helical edge states are confined along domain walls that separate regions of opposite mass $g$. Here, we can simply tune the mass $g$ by changing the radius of the central snowflake, see Fig. 2. As discussed above when all snowflakes have the same radius (corresponding to $\Delta r = 0$) the $p$- and $d$- bands are degenerate at the Γ point ($g = 0$). For a decreased (increased) radius $r_c$ of the central snowflakes, the $d$-orbitals have larger (smaller) energy, corresponding to a positive (negative) mass $g$, cf. Fig. 2. In order to understand this behavior, it is useful to observe that the $p$-orbitals have extra nodes at the external links leading out of the (enlarged) unit cell, enforced by a phase-difference of $\pi$ across those links. When all snowflakes have equal radius, the additional energy cost associated with the larger phase gradient (compared to a $d$-orbital) across these external links exactly offsets the benefit of a reduced phase gradient on a path encircling the central snowflake. Obviously, stronger (weaker) internal links [corresponding to a decreased (increased) central snowflake radius $r_c$] favor energetically the $p$- ($d$-) states, eventually leading to the behavior displayed in Fig. 2.

Strip in the continuum model. – To ascertain the appearance of edge states at an interface with a band inversion, we first consider a strip configuration with a mass term $g(y)$ varying along the transverse (finite) $y$-direction from $-g_0$ to $+g_0$. We employ the continuum limit based on Eq. 4, using the envelope function approximation. Following this standard procedure, we obtain a right (left) moving state, with a linear dispersion $E =vk_x$ ($E = -vk_x$) for $s = +1$ ($s = -1$), that decays exponentially away from the domain wall, with a penetration depth $\xi = v/g_0$. This behaviour, obtained in the continuum limit, is confirmed in direct finite-element simulations of the microscopic equations of elasticity for a strip geometry.

Helical edge channels in finite-element simulations. – We will now verify the above statements for the snowflake crystal, using the full microscopic acoustic equations. For that purpose, we consider a strip with a finite extent along $y$. Before we investigate the effects of domain walls, we first briefly discuss the strip with a spatially homogeneous mass term, i.e. composed of the hexagonal building blocks comprising three snowflakes (Fig. 1a, red shaded area), with the central snowflake’s radius deviating by...
\( \Delta r \). Figure 3 shows the band structures of strip configurations with \( \Delta r = -200 \text{ nm} \) (b) and \( \Delta r = 200 \text{ nm} \) (c), obtained by the COMSOL finite element solver. The Dirac cones are replaced by a complete bulk band gap. There are states that appear in addition to the bulk-derived bands and that are localized at the boundaries (Figure 3d), arising due to the symmetry-breaking at these sharp sample boundaries. These edge states are not protected by any symmetry and are highly sensitive to the exact geometry of the edge. Moreover, they are two-fold degenerate; one state is localized at the upper and the other at the lower boundary.

Next, we attach both structures to each other (Fig. 3k) and obtain a strip geometry with a domain wall where the sign of the mass term \( g \sim \Delta r \) flips. The corresponding band structure is shown in figure 3l, which is basically a superposition of the band structures of the bare strips with \( \Delta r = \pm 200 \text{ nm} \). However, in addition to the bulk bands and the afore-mentioned states at the sample boundaries, two states appear that traverse the gap entirely, with a linear dispersion of opposite slope (group velocity). Moreover, there is no discernible avoided crossing between these two states, underlining the absence of back-scattering expected for topological insulators due to the symmetry-protection. Figure 3m shows the quasi-momentum resolved wave function of the right-moving state (red energy dispersion in panel d). For small quasi-momenta it is highly confined around the domain wall, with a typical penetration depth inversely proportional to the size of the bulk band gap (as expected from \( \xi = v / \xi_0 \) derived in the continuum model).

**Effects of disorder.** The engineered symmetry \( \tilde{S} \) will not protect against completely arbitrary (generic) disorder. This behaviour is in fact common to all bosonic topological insulators [30]. However, \( \tilde{S} \) is valid near the \( \Gamma \)-point. Therefore, generically speaking, one may expect that this protection is preserved near smooth defects, interfaces, and sample boundaries, which admit only wavevectors close to \( \Gamma \). On top of this, even for sharp domain boundaries, we find in the full finite-element simulations that there is no discernible back-scattering for the parameters we have explored. Such a scattering would show up in the form of a minigap, i.e. an avoided crossing between the counterpropagating edge states. This unexpected robustness in the presence of sharp interfaces has been observed as well in works analyzing photonic structures based on \( C_6 \) symmetry [24, 25]. Moreover, one can show that even short-range defects of a certain kind, that are compatible with the symmetry \( \tilde{S} \), do not induce scattering between counterpropagating edge states. For example, both of the following perturbations have zero matrix element between sectors of opposite helicity: changing the masses of all 6 triangles in a given unit cell by the same amount, or leaving out a single snowflake hole.

**Arbitrary boundaries.** We now consider a finite system with an arbitrarily shaped boundary to observe unidirectional transport of mechanical excitations and the effects of disorder. To keep the computational effort manageable, we approximate the snowflake crystal by a tight-binding model, where the sites of this model directly correspond to the physical triangles that are arranged in a honeycomb lattice. Note that in order to obtain most of the insights we are aiming for here, it would be more generally sufficient to use any tight-binding model that exhibits the same symmetries that underlie the topological protection in our system. We use a hexagonal unit cell comprising six sites with equal eigenfrequencies. To mimic the mass term, hopping rates within a unit cell, \( J \), deviate from hopping rates between different unit cells, \( J \). Again there is a direct interpretation: By changing the radius of the central snowflake in the real microscopic structure, the links connecting the triangles also change, consequently leading to different coupling between two triangles.

As shown above, the unidirectional edge states are superpositions of the states with the same helicity \( s \) (e.g. \( p^+ \) and \( d^+ \)). Figure 4 shows the energy distribution for a mechanical wave that is propagating at the domain wall between two domains with different mass terms. We excite a whole unit cell (indicated by the yellow arrow) with a \( |p^-\rangle \)-type mode shape, thereby launching a sound wave that just propagates to the right. By calculating
the linear response of each lattice site to this particular excitation, we obtain the propagation probability (modulus squared of the Green’s function) of the mechanical excitation. As mentioned in the general discussion near Eq. (4) the symmetry $\hat{S}$ is obeyed to a very good approximation within a rather large fraction of the Brillouin zone. As a consequence, any remaining admixture of the opposite helicity is quickly suppressed when a sharp domain wall (with a sudden jump in hopping amplitudes) is replaced by even only a slightly smoothed wall. This is confirmed by the numerical simulations displayed in Fig. [4].

**Conclusions.** – The snowflake topological insulator for sound waves proposed here is straightforward to fabricate at any scale, down to the nanoscale. It can be excited and read-out using a variety of different approaches, including electrical, mechanical, and optomechanical (adapting the ideas presented in [23]). The simplicity of the nanoscale design (and the small dimensions of the unit cell) will turn such a modified snowflake crystal into a versatile platform for generating arbitrary phononic circuits and networks [31,32] on the chip, which may couple to hybrid quantum systems of various kinds and could also contain optically tuneable non-reciprocal elements [33].

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