Realizing and manipulating space-time inversion symmetric topological semimetal bands with superconducting quantum circuits

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We have experimentally realized novel space-time inversion (P-T) invariant $\mathbb{Z}_2$-type topological semimetal-bands, via an analogy between the momentum space and a controllable parameter space in superconducting quantum circuits. By measuring the whole energy spectrum of system, we imaged clearly an exotic tunable gapless band structure of topological semimetals. Two topological quantum phase transitions from a topological semimetal to two kinds of insulators can be manipulated by continuously tuning the different parameters in the experimental setup, one of which captures the $\mathbb{Z}_2$ topology of the PT semimetal via merging a pair of nontrivial $\mathbb{Z}_2$ Dirac points. Remarkably, the topological robustness was demonstrated unambiguously, by adding a perturbation that breaks only the individual $T$ and $P$ symmetries but keeps the joint PT symmetry. In contrast, when another kind of PT-violated perturbation is introduced, a topologically trivial insulator gap is fully opened.

Symmetry and topology, as the two fundamentally important concepts in physics and mathematics, have not only manifested themselves in science, but also provided us profound understanding of arresting natural phenomena. Recently, topological gapless systems, such as Weyl semimetals and a variety of Dirac semimetals, as well as $\mathbb{Z}_2$ topological metals/semimetals, have significantly stimulated research interest. Analogous to that in gapped topological systems such as topological insulators and superconductors, the discrete symmetry that is rather robust against symmetry-preserved perturbations can enrich the topological physics of gapless systems as well. As is known, the discrete time-reversal ($T$), space-inversion ($P$), and charge-conjugate ($C$) symmetries are fundamental and intriguing in nature. For examples, in high energy physics, any local quantum field theory must preserve the joint CPT symmetry, which is required by the unitarity and Lorentz invariance of the theory, and the source of CP violation still remains as one of seminal mysteries in the Standard Model. While in condensed matter systems, it is ubiquitous that $P$, $T$, and $C$ put the constraints on band structures and lead to new topological classifications of band theories. Among various combinations of $P$, $T$, and $C$, the joint PT symmetry actually inverts the space-time coordinates $x^\mu \rightarrow -x^\mu$ with $\mu = 0, 1, 2, 3$ and $x^0 = t$, and therefore evidences itself to be fundamental and significant in physics. Very recently, a theory of PT-invariant topological gapless bands has rigorously been established, through revealing a profound connection between the PT symmetry and an elegant KO theory of algebraic topology. On the other hand, it is noted that artificial superconducting quantum circuits possess high controllability, providing a powerful and ideal tool to quantum-simulate and explore novel quantum systems, including topological ones.

In this Letter, we have realized experimentally the novel PT symmetry-protected topological semimetal-bands that represent a gapless spectrum on a square-lattice, via an analogy between the momentum space and a controllable parameter space in superconducting quantum circuits. By measuring the whole energy spectrum of our system, we have imaged clearly an exotic tunable gapless band structure of topological semimetals, shown as nontrivial $\mathbb{Z}_2$-type Dirac points in momentum space. The two new distinct quantum phase transitions from a topological semimetal to two different insulators can be manipulated by continuously tuning the different parameters in the simulated effective Hamiltonian, particularly one of which exhibits the $\mathbb{Z}_2$ topology in the PT semimetal via merging a pair of nontrivial $\mathbb{Z}_2$ Dirac points. Furthermore, to demonstrate unambiguously the topological robustness of PT symmetry, a perturbation that breaks only the individual $T$ and $P$ symmetries is intentionally added, with the joint PT symmetry being still preserved. It is verified by experimental data that the Dirac points of the topological semimetal-bands still present under such perturbations, though the point positions and the band pattern are changed drastically. In a sharp contrast, when another kind of perturbation is added to break the PT symmetry in our experiment, the energy gap is fully opened and the Dirac points disappear completely, showing the essential role of PT symmetry underlying the topological robustness. All of these illustrate convincingly the topological protection of PT semimetals. Notably, the present work is the first experimental realization and manipulation of fundamental space-time inversion symmetric topological semimetal-
bands (without individual $T$ and $P$ symmetries) in nature, which opens a window for simulating and manipulating topological quantum matter.

The physical manifestation of $PT$ symmetry in band theories can simply be seen from the commutation relation as $[\hat{A}, H] = 0$, where $H$ is the system Hamiltonian, and the joint $PT$ symmetry is represented by an anti-unitary operator $\hat{A}$. When $\hat{A}^2 = 1$, the topological classification of band-crossing points in two-dimensional band structures corresponds to the reduced $KO$ group, $KO(S^1) \cong \mathbb{Z}_2$, which implies that there exist band-crossing points having nontrivial $\mathbb{Z}_2$ topological charges in two dimensions \[17\]. Although the $KO$ theory of algebraic topology seems to be rather abstruse for most physicists, the predicted topological band crossing points can be realized in a simple but representative dimensionless Hamiltonian, which is explicitly given by \[17\]

$$H(k) = \sin k_x \sigma_2 + (\lambda \pm \cos k_y) \sigma_3$$  \hspace{1cm} (1)

with the $PT$ being denoted by $\hat{A} = \sigma_3 \hat{K}$, where $\sigma_j$ is the $j$th Pauli matrix, and $\hat{K}$ denotes the complex conjugate operation. When $-1 < \lambda < 1$, the model \[1\], which describes actually a topologically nontrivial spin(1/2)-orbital quantum system in two dimension, has four band-crossing points possessing the $PT$-protected $\mathbb{Z}_2$ ($\nu_{\mathbb{Z}_2} = 1$) topological charges. It is noted that although the model \[1\] has both $\hat{P} = \sigma_3 \hat{I}$ and $\hat{T} = \hat{K} \hat{I}$ symmetries with $\hat{I}$ being the inversion of the wave vector $k$, the topological stability of these band-crossing points merely requires the joint $PT$ symmetry according to the $PT$ invariant topological band theory, namely, the $T/P$-symmetry is allowed to be broken individually while the $PT$ topological protection still remains.

Experimental demonstration of this new kind of symmetry protected topological gapless band will significantly deepen our understanding of topological quantum matter. However, there are several big challenges that hinder the realization and investigation of the topological properties of this kind of Hamiltonians in real condensed matter systems. The first is how to synthesize the materials with a designated Hamiltonian. Secondly, even if one is fortunate enough to have such kind of real materials, it seems extremely hard to tune the parameters continuously for studying fruitful topological properties including various topological quantum phase transitions. Moreover, it is quite difficult in experiments to directly image the whole momentum-dependent electronic energy spectrum of a bulk condensed matter system, noting that only a part of electronic spectra (or information of Fermi surfaces/points) may be inferred from the angle-resolved photoemission spectroscopy data (or quantum oscillation measurements). Therefore, it is imperative and important as well as significant to use artificial quantum systems like superconducting quantum circuits to simulate $H(k)$ faithfully and to explore topological properties of the system. Below we will realize the Hamiltonian of Eq.\[1\] in the parameter (analogous to the momentum) space via implementing a kind of fully controllable quantum superconducting circuits, such that the band structure can directly be measured over the whole first Brillouin zone (BZ) of square lattices, enabling us to demonstrate the unique topological nature of the corresponding semimetal-bands and to clearly visualize some crucial properties.

![Figure 1: Experimental scheme for the realization of the lattice Hamiltonian.](image)

a. States $|2\rangle$ and $|1\rangle$ of a transmon are used as the energy levels of an artificial spin-1/2 particle, whose three components may be denoted by the three Pauli matrices $\hat{\sigma}_{1,2,3}$. $|0\rangle$ is chosen as an ancillary level to probe the eigenvalues of a Hamiltonian. Microwaves with various frequencies, phases, and amplitude are applied for the construction of a semimetal Hamiltonian and circuit QED readout, respectively. \[20\]. b. The constructed Hamiltonian is implemented with modulation of microwave amplitude, frequency, and phase, mapping to the momentum space of a square lattice.
The two states \(|\psi_0\rangle\) and \(|\psi_1\rangle\) correspond to the frequency of Rabi oscillations along X (Y) axis on the Bloch sphere, which is continuously adjustable by changing the amplitude and phase of microwave applied to the system. The Hamiltonian of the qubit in the rotating frame is given by:

\[
\hat{H} = \sum_{i=1}^{3} \Omega_i \sigma_i / 2, \tag{2}
\]

where \(\Omega_1\) (\(\Omega_2\)) corresponds to the frequency of Rabi oscillations along X (Y) axis on the Bloch sphere, which is continuously adjustable by changing the amplitude and phase of microwave applied to the system. \(\Omega_3 = \omega_{21} - \omega\), is determined by the detuning between the system energy level spacing \(\omega_{21}\) and microwave frequency \(\omega\). By carefully designing the waveform of AWG, we can control the frequency, amplitude, and phase of microwave. In our experiment, we first calibrated the parameters \(\Omega_1\), \(\Omega_2\), and \(\Omega_3\) using Rabi oscillations and Ramsey fringes, and then designed the microwave amplitude, frequency and phase to let \(\Omega_1 = 0\), \(\Omega_2(k_x) = \Omega \sin k_x\), \(\Omega_3(k_y) = \lambda \Omega + \Omega \cos k_y\), with \(\Omega = 10\) MHz being chosen as the energy unit.

The measured energy spectrum of a typical space-time inversion invariant topological semimetal. a, Three-dimensional plot of the band structure of spectroscopy measurement. By tuning the driving amplitude, frequency, and phase gradually, we image the band structure of the system in the momentum space point by point. b, Magnitude of energy gap obtained from direct measurements of the energy spectrum of the system as function of \(k_x\) and \(k_y\) in the first BZ. Four nontrivial Z2-type Dirac points located inside the bright regions can be observed at \((0, \pm \pi/2), (\pi, \pm \pi/2)\), in full agreement with the theoretical prediction.
Whenever the process of merging and annihilation of the discharged \[17\]. In agreement with the theoretical pre-

logical protection, which requires the PT symmetry, is distorted drastically, showing the robust of the topological

nature protected by the PT symmetry. Top and bottom panels correspond respectively to the cases of \( \eta = 0 \) and \( \eta = 0.5 \) on the plane of \( k_x = \pi/2 \). The bright yellow and dashed green lines denote the experimental data and theoretical cal-

culations from Eq.(1) with \( H_1^l \) being added, respectively. b, Whenever the PT symmetry is broken by adding the term \( H_2^l = \varepsilon \sigma_1 \) with a constant \( \varepsilon \) (\( \sim 0.5\Omega \)), a gap is fully opened. Here \( \lambda = 0 \) for both (a) and (b).

Figure 3: Symmetry-related topological features of the Dirac points for two different but representative kinds of perturbations. a, When \( H_1^l = \eta \sigma_2 \) is added with \( \eta = 0.5 \) in unit of \( \Omega \), which breaks both \( T \) and \( P \) but preserves the PT symmetry, Dirac-like points still exist, though the gapless point positions are shifted (marked by the green square) and the band pattern is distorted drastically, showing the robust of the topological nature protected by the PT symmetry. Top and bottom panels correspond respectively to the cases of \( \eta = 0 \) and \( \eta = 0.5 \) on the plane of \( k_x = \pi/2 \). The bright yellow and dashed green lines denote the experimental data and theoretical cal-

culations from Eq.(1) with \( H_1^l \) being added, respectively. b, Whenever the PT symmetry is broken by adding the term \( H_2^l = \varepsilon \sigma_1 \) with a constant \( \varepsilon \) (\( \sim 0.5\Omega \)), a gap is fully opened. Here \( \lambda = 0 \) for both (a) and (b).

Figure 4: Quantum phase transitions from a topological gapless semimetal to a gapped insulator as changing parameter \( \lambda \). a, Spectroscopy at \( k_x \approx 0 \) for various \( \lambda \). From right to left \( \lambda \) are 0, 0.5, 1 and 1.5, respectively. It is seen that when \( \lambda \) is increased from 0 to 1, then larger than 1, the number of Dirac-like points decreases from 4, to 2, then to 0, where the gap gradually is opened, demonstrating that a topological PT invariant semimetal phase transits to a normal insulator phase. b, Magnitude of minimum energy gap \( E_g \) in the first Brillouin zone as a function of \( \lambda \), as predicted theoretically from Eq.(1).

As shown in Fig.4b, we continuously increase the parameter \( \lambda \) from 0 to 2. Starting from \( \lambda = 0 \), where two band-crossing points are well separated at \( k_y = \pi/2 \) and \( -\pi/2 \), respectively, in the one-dimensional subsys-


tem with \( k_x = 0 \), the two band-crossing points are gradually moving closer and closer to each other (with re-

gard to their distances to the BZ boundaries) when \( \lambda \) is increased smoothly, then they are merged to be a new band-crossing point at the edge of the first BZ for \( \lambda = 1 \), which should be a topologically trivial point according to the topological band theory as mentioned above. Indeed, when \( \lambda \) is further increased to be bigger than 1, it is observed that the band crossing point of a trivial topological charge is gapped out, leading to a topologically trivial insulator that has even the PT symmetry [41], which verifies the aforementioned theoretical prediction.

To summarize, we have reported the first experimental realization and manipulation of fundamental space-time inversion invariant topological semimetal bands possessing neither \( T \) nor \( P \) symmetry. The non-trivial bulk topological band structures of PT symmetry have directly been imaged with superconducting quantum circuits. Moreover, two exotic topological quantum phase transitions have been observed for the first time. The present work is expected to stimulate a huge experimental and theoretical interest on various PT symmetric topological metals/semimetals, paving the way for quantum-simulating novel topological quantum materials.

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41 The triviality follows from the same argument as that in Ref. 10, but for the infinite limit of $\lambda\pi_3$. 

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