Realization of the Single-pair-Weyl Phonons with the Maximum Charge Number in Acoustic Crystals

Zhe-Qi Wang,† Qing-Bo Liu,† Xiang-Feng Yang,† and Hua-Hua Fu†,‡

†School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan 430074, China.
‡Institute for Quantum Science and Engineering, Huazhong University of Science and Technology, Wuhan, Hubei 430074, China.

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To observe the Weyl phonon (WP) with the maximum charge and to design a realistic material structure containing only single-pair-WPs have long been considered two challenges in the field of topology physics. Here we have successfully designed an acoustic crystal to realize the single-pair-WPs with the maximum charge for the first time. Our theoretical simulations on acoustic band dispersions demonstrate that protected by the time-reversal symmetry (T) and the point group symmetries, a WP with the charge -4 (C = -4) and another WP with C = +4 are located at the high-symmetry point Γ and R, respectively, with the absence of any other kinds of WPs. Moreover, the single-pair-WPs obtained here are designed by the simplest two-band mode, and the related quadruple-helicoid Fermi arcs can be observed clearly in experiments, since they aren’t covered by any bulk bands and hybridized by other kinds of WPs. Our theoretical results provide a reliable acoustic crystal to study the topological properties of the single-pair-WPs with the maximum charge for experimentalists in this field.

Introduction. We well know that to discover new kind of Weyl phonons (WPs) has been regarded as one of central topics in the field of topology physics [1–10]. Owing to the protections from different symmetries in materials and band degeneracies, single WPs with Chern number ±1, double WPs with Chern number ±2, triple WPs with Chern number ±3 [11] and other WPs characterized by different charges have been defined in theory [12], and some of them have been confirmed successfully in experiments [13]. Due to the compensation effect from the Nielsen-Ninomiya no-go theorem [16], these WPs exhibit exotic nontrivial surface states, including long surface arcs and double-helicoid arc states in surfaces Brillouin zone (BZ) [13]. Very recently, it has been established that the charge numbers in WPs exist an upper limit and their maximum charge number should be four (|C| = 4). For example, a recent work demonstrated that at the twofold degenerated band crossings with C3 screw symmetry in electronic systems, if the cubic symmetry is taken into account further, the twofold Weyl points may reach the maximum charge number of ±4 [17]. In our previous work, the WPs with the maximum charge number exist in the chiral crystal samples of BiIrSe and Li3CuS2 [18]. However, how to observe clearly the WPs with the maximum charge and the associated quadruple-helicoid surface arcs without the compensations from other kinds of WPs has still been a hard task in experiments.

On the other side, the realization of single-pair-WPs in phononic systems has also been regarded as another challenge in the field of topology physics, because the single-pair-WPs are helpful to uncover new topological phenomena [19], although single-pair Weyl points have been observed in some magnetic materials [20–23]. “Single-pair” defined here refers to the minimal number of WPs which should appear in a topological crystal under the requirement of no-go theorem. It is inspiring that if a WP is considered to compensate with other kinds of WP hosting different charge numbers, the minimal of WPs in the first BZ of a realistic material example may reach three. For example, the symmetry-protected topological triangular WP complex have been proposed in α-SiO2 [24] and in SrSi2 [25]. This kind of Weyl complex are composed of three WPs, i.e., two single WPs with C = -1 and one double WP with C = +2, to ensure the total topological charge neutrality of the BZ. However, a single-pair-WPs with the maximum charge haven’t been observed in any realistic material example in experiments up to date.

To deal with the above two thorny issues, in this work, we have designed theoretically a three-dimensional (3D) acoustic crystal with cubic symmetries, displaying the space group (SG) with No. 207 [20]. Our theoretical simulations on the band dispersions of this acoustic crystal demonstrate that a WP with C = -4 and another WP with C = +4 are located at the high-symmetry points Γ and R, respectively, which are confirmed further by the Chern number calculations and the symmetry analysis. More importantly, apart from these two WPs, no any other kinds of WPs exist in the first BZ, indicating that we have successfully realized the single-pair-WPs with the maximum charge in acoustic crystals for the first time. Moreover, the single-pair-WPs obtained here possess their unique advantages: (i) The nontrivial bands to construct the WPs are composed only by two nontrivial bands, which can be considered as the simplest band model to realize the single-pair-WPs with the maximum charge. (ii) Since the WPs aren’t compensated with other kinds of WPs with different charges and the related nontrivial bands aren’t covered by any other bulk acoustic
bands, the related quadruple-helicoid surface arc states can be observed clearly in experiments. Therefore, our theoretical results put forwards an ideal crystal structure to study the topology physics of the single-pair-WPs with the maximum charge.

**Structural design of 3D acoustic crystal.** The 3D acoustic crystal designed here has a cubic unit cell with the lattice constant \( a = 10 \) cm as drawn in Figs. 1(a) and 1(b). Each unit cell contains an embellished Helmholtz resonator and six (eight) thin tubes colored by blue (yellow) are adopted to simulate the nearest (third) neighboring couplings. For the nearest neighboring coupling, we chose the position parameter as \( l_1 = 0.3a_1 \) and the radius of the coupled tube as \( r_1 = 0.023a_1 \) [see Fig. 1(c)], while for the third neighboring coupling, the corresponding parameters are set as \( l_2 = 0.1\sqrt{2}a_1 \) and \( r_2 = 0.024a_1 \) [see Fig. 1(d)]. Meanwhile, the tubes for the nearest (third) neighboring coupling are composed of four-(three-)tube-based helical couplings, and their helicity angle is set as \( \theta_1 = 90^\circ \) (\( \theta_2 = 60^\circ \)). By modifying the structural parameters [see details in Supplemental Material (SM) [27]], we can obtain the acoustic states we want to gain. For example, as the distance between two nearest faces is set as \( d_1 = 0.55a_1 \), two special states \( \{2x^2 - x^2 - y^2\} \) and \( |\sqrt{3}(x^2 - y^2)| \) in \( d \) orbital are generated to form square-relation band dispersions at the high-symmetry points \( \Gamma \) and \( R \), which build the curial three acoustic bands to construct the WPs with the maximum charge number. For this case, the detailed structural parameters for the connections between the coupled tubes and the resonator are described in Fig. S1(c)-S1(f) in SM [27]. Note that the acoustic crystal designed here can be fabricated easily by the 3D-printing technology on photosensitive resin.

**Symmetry analysis and stimulation method.** To study the topological features of the WPs with \( C = \pm 4 \) in the acoustic crystal constructed here, we firstly establish an effective \( k \cdot p \) model. Considering that the high-symmetry point \( \Gamma \) in SG with No. 207 belongs to the little group \( O_h \), the related symmetry operators include one three-fold rotation symmetry \( \{C_{31}^- \{000\}\} \), three two-fold rotation symmetries \( \{C_{2z} \{000\}\} \), \( \{C_{2z} \{00\}\} \) and \( \{C_{2z} \{00\}\} \) and \( T \). Besides, the WP at this point is protected also by the 2D irrep, i.e., \( \Gamma_3 [26] \). Thus, on the basic vectors of \( \{2x^2 - x^2 - y^2\}, \{\sqrt{3}(x^2 - y^2)\} \), the representation matrices for them can be written as

\[
C_{31}^+ = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}, C_{31}^- : xyz \mapsto yzx
\]

\[
C_{2x} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, C_{2z} = C_{2z}.
\]

\[
C_{2z} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \sigma_z, C_{2a} : xyz \mapsto xy\bar{z}; T = K.
\]

Under the above operations, the final \((k \cdot p)\)-invariant
Hamiltonian can be derived as,
\[ H(q_x, q_y, q_z) = a_1(q_x^2 - q_y^2)\sigma_x + a_2q_xq_yq_z\sigma_y + \frac{a_1}{\sqrt{3}}(q_x^2 + q_y^2 - 2q_z^2)\sigma_z. \]

Obviously, the above two-band \( k \cdot p \) Hamiltonian demonstrates that along the [111] direction, the dispersions display a \( k^3 \)-type feature, while along other directions in the phonon bands, a \( k^2 \)-type feature, supporting the existence of the WP with \( C = -4 \) at the point \( \Gamma \). Note that the above \( k \cdot p \) model is also applicable at the point \( R \).

The band dispersions of 3D acoustic crystal designed here are calculated by the commercial software COMSOL Multiphysics (Pressure Acoustic module). In our simulations, the air density and sound speed are set as 1.18 kg m\(^{-3}\) and 343 m s\(^{-1}\), respectively. All air-solid interfaces are applied along the edges of unit cell. For the surface band dispersions, the Floquet periodic boundary condition is adopted both in the \( x \)- and \( y \)-directions, while the hard acoustic boundary condition is adopted in the \( z \)-direction of the supercell with the size of \( 1 \times 1 \times 15 \).

Chern numbers or topological charge of WPs are calculated by the Wilson loop method \[28, 29\].

Topological features of single-pair WPs with \( C = \pm 4 \) In what follows, we turn to examine the unique nontrivial features of the single-pair-WPs with \( C = \pm 4 \) in the present acoustic crystal. Firstly, the acoustic band dispersions along high-symmetry paths [see Fig. 1(e)] are gained and illustrated in Fig. 1(f). One may find that there are two band crossings located at the high-symmetry points \( \Gamma \) and \( R \) in the frequency region \( 3.75 < f < 3.9 \) KHz (see the grey box). Moreover, around the above two points, the bands display as \( k^3 \)-relation dispersions along the high-symmetry directions, which is well consistent with the analysis results from the \( k \cdot p \) model. Moreover, our simulations show that the above acoustic bands host nonzero Chern numbers \( \pm 4 \), and their states described by acoustic pressure (\( p \), profiles) are contributed only by two acoustic basic states \( \varphi_1 = |2z^2 - x^2 - y^2 \rangle \) and \( \varphi_2 = |\sqrt{3}(x^2 - y^2) \rangle \), as described in Figs. 1(g) and 1(h). Therefore, the degenerate acoustic bands clearly demonstrate that two WPs with
\( C = \pm 4 \) are located at the points \( \Gamma \) and \( R \) in the first BZ as described in Fig. 2(a), which are verified further by the evolutions of the average positions of Wannier centers, as illustrated in Figs. 2(c) and 2(d).

Particularly, apart from the above two WPs in the first BZ, we haven’t found any other kind of WPs existing in the present acoustic crystal and meanwhile, these two WPs with \( C = \pm 4 \) obtained here are also constrained strictly by the no-go theorem [10]. It should be stressed that in almost all previous works to design and realize the WPs with the maximum charge whether in electronic or in phononic systems [30–34], including two very recent experimental works to observe the WP with \( C = -4 \) in photonic crystals [35] and the WP with \( C = +4 \) in phononic crystals [36], only one WP with the maximum charge has been achieved and is compensated with the hybrid-WPs with the charges \( |C| = 1 \) or \( |C| = 2 \). Therefore, it can be believed that the acoustic crystal designed here can be regarded as the first crystal structure to realize the single-pair-WPs with the maximum charge.

Furthermore, in comparison with the WP with \( C = \pm 4 \) reported previously, the single-pair-WPs with the maximum charge achieved here possess several unique advantages. Firstly, the single-pair-WPs in the first BZ aren’t hybridized or compensated by other kinds of WPs characterized by different charge number, which are helpful for us to grasp and study the main topology physics of the WPs with the maximum charge. Secondly, the single-pair-WPs are located nearly at the same acoustic frequencies and not covered by other bulk acoustic bands, indicating the two WPs can be detected easily in experiments and meanwhile, the corresponding quadruple-helicoid surface arc states may be observed clearly in the related surfaces BZ. Thirdly, in all previous structures to realize the WPs with \( C = \pm 4 \), the topologically acoustic bands are composed of at least three basic band modes. However, the topological bands to construct the single-pair-WPs with maximum charge number here are
comprised only by two band modes as described in Figs. 1(f) and 1(g). Moreover, by adjusting the air resonator structure and the connection of coupling tube (see details in Supplemental Material), the above excitation states are clearly distinguished from the three $p$ states ($p_x, p_y, p_z$) and other three $d$ states ($d_{xy}, d_{xz}, d_{yz}$). Therefore, we have successfully constructed the single-pair-WPs with the maximum charge by the simplest two-band model in our acoustic crystal design.

Quadruple-helicoid surface arcs of single-pair WPs with $C = \pm 4$. To confirm the inspiring topologically nontrivial features of the single-pair-WPs hosting the maximum charge number, we study further their acoustic surface states. As a defining feature of Weyl semimetals [37-40], the presence of topological surface states has been considered as smoking gun evidence for their topologically nontrivial properties, which provides us an effective way to identify the topological charge of a bulk WP by examining the surface arcs along a closed loop encircling its projected WP. In the present acoustic crystal, the band dispersions in a tube orientated in the $k_z$-direction of 3D BZ reflect the well-defined Chern numbers. Considering the bulk-edge projection relation, if the metacrystal is terminated at the $k_z$-$k_y$ surface, the chirality of topological surface states along the tube-projected loop gives the Chern numbers of the associated 2D band gaps, from which one may deduce the total topological charge of the WPs inside. Particularly, if there is only one node inside the tube, its topological charge can be determined directly by the overall chirality of topological surface states. Following these derivations, the projected bulk dispersions along the high-symmetry paths $X$-$M$-$\Gamma$-$\overline{X}$ in the $k_x$-$k_y$ plane [i.e., the blue plane in Fig. 3(a)] are drawn in Fig. 3(b), in which the topological surface states (highlighted by the red color) are distinguished from the bulk states, especially in the front two paths. In Figs. 3(c) and 3(d), we give the surface-projected dispersion along a small loop (of radius $0.5\pi/a$) centered at $\Gamma$ and $\overline{M}$. Evidently, four gapless surface states with overall positively and negative slopes traverse clearly the full gap between the lowest and highest projected bands, confirming further that the WPs possess the topological charges of $\pm 4$. Note that the property that the surface states of the WPs with $C = \pm 4$ show opposite signs in slopes, and the fact that they together with their neighbouring bulk states display antisymmetric behaviors have been verified for the first time in a realistic acoustic crystal.

The topological charges of the WPs and their inspiring topological features can be verified from the surface iso-frequency contours ranging from 3.81 KHz to 3.84 KHz. Firstly, the 2D acoustic dispersions in this frequency region around the points $\Gamma$ and $R$ are shown in Fig. 4(a) and 4(b), respectively, where four screw surfaces, i.e., the quadruple helicoid surface states, display

![Diagram](image_url)
clearly around these two points in the $k_x - k_y$ plane. Moreover, the chirality of the helicoid reflects the chirality of the WPs with different charge numbers [41]. For example, by increasing the acoustic frequency, the four surface arcs clockwise wind around the point $\bar{\Gamma}$, whereas they anticlockwise wind around the point $\bar{\Gamma}$, which show that the helicoids around the points $\bar{\Gamma}$ and $\bar{\Gamma}$ have opposite chirality, which are in good agreement with the chirality of the WPs with $\pm 4$, and well consistent with the previous analysis result gained from the simplified lattice model in electronic systems [43]. To demonstrate further this property, the evolutions of quadruple helicoid surface arcs around the points $\bar{\Gamma}$ and $\bar{\Gamma}$ are simulated with decreasing frequency in Figs. 4(c)~4(h), in which several unique properties are uncovered: (i) the four projections of quadruple helicoid surface arcs show clearly, verifying further their maximum charge number of $\pm 4$; (ii) their opposite chirality displays clearly in Figs. 4(c) and 4(f); (iii) the Lifshitz transition occurs clearly around two projected points $\bar{\Gamma}$ and (iv), the quadruple helicoid surface arcs aren’t covered by any trivial mode, indicating that they and related transition can be observed clearly in experiments.

**Conclusion.** Through designing an acoustic crystal, we have successfully achieved single-pair WPs with the maximum charge numbers for the first time. Our theoretical simulations demonstrate that the WPs with $\pm 4$ are localized at the high-symmetry points $\Gamma$ and $\bar{R}$ in the first BZ and follow strictly the no-go theorem, and aren’t hybridized or compensated by other kinds of WP with different charges. The WPs with $C = \pm 4$ obtained here possess the opposite chirality and the projected bulk dispersions display clearly quadruple-helicoid surface arc states. Moreover, in our structure design of acoustic crystal, we have realized the single-pair-WPs with the maximum charge by the simplest two-band model, in comparison with the past designs with no less than three bands reported previously. Particularity, the all size parameters adopted in the acoustic crystal are provided in details and can be fabricated easily by the present 3D-printed technology, indicating the single-pair-WPs with the maximum charge number and the unique quadruple-helicoid surface arc states can be detected easily in experiments. Our findings not only realize the single-pair-WPs with the maximum charge, but also provide realistic acoustic structure to study their topology physics.

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*hhfr@hust.edu.cn

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