Realizing and detecting the fundamental Weyl semimetal phase

Yue-Hui Lu,1, 2 Bao-Zong Wang,3, 1 and Xiong-Jun Liu1, 2, 4, 5

1 International Center for Quantum Materials and School of Physics, Peking University, Beijing, China 100871
2 Collaborative Innovation Center of Quantum Matter, Beijing 100871, China
3 Shanghai Branch, National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, University of Science and Technology of China, Shanghai 200331, China
4 Beijing Academy of Quantum Information Science, Beijing 100193, China
5 CAS Center for Excellence in Topological Quantum Computation, University of Chinese Academy of Sciences, Beijing 100190, China

There is an immense effort in search for various types of Weyl semimetals, of which the most fundamental phase consists of the minimal number of, i.e. two Weyl points. Such fundamental Weyl phase is of peculiar importance and, however, has not been observed due to the lack of reliable quantum material or feasible scheme for the realization and detection. Here we solve the existing challenges and demonstrate how the fundamental Weyl semimetal is realized with a maneuverable optical Raman lattice which is completely accessible in the experiment. Moreover, we propose the highly feasible technique to resolve the 3D band topology of the Weyl semimetal via only 2D measurements, with which the configuration of Weyl points can be precisely identified. This work is leading to the realization and detection of the most fundamental phase in Weyl semimetal family.

Introduction. Weyl fermion, as a cousin of photon, is a massless particle with definite chirality [1]. While it has not been identified as a fundamental particle in nature, the Weyl fermion can emerge as low energy quasiparticle in the Weyl semimetals, which have been widely observed in solid state matter [2–5], also meta-material [6–8], and generated considerable interests in the recent years [9]. In the crystal the Fermion doubling ensures that the Weyl points come in pairs, with two Weyl nodes in each pair having opposite chiralities [10, 11]. Thus the minimal number of Weyl points in a semimetal is two, and such minimal case renders the most fundamental phase in the Weyl semimetal family, dubbed the fundamental Weyl semimetal (FWS) for convenience. The Weyl nodes in the FWS are not symmetry-related, and all basic symmetries in the FWS can be broken [9].

The FWS phase has peculiar importance compared with other Weyl phases with more Weyl points. As protected sonly by chiral Chern numbers, the two Weyl nodes of opposite chiralities [12] in the FWS cannot be trivially gapped out by perturbations or interactions. This leads to an important consequence that any interacting phase born from FWS has to be topologically nontrivial, being either gapless with new topological Weyl points, or gapped with exotic bulk topology. For example, the superconducting phase with pairing between two different Weyl cones gives a gapless Weyl superconductor [13–16]. Further, the Fulde-Ferrell-Larkin-Ovchinnikov pairing order within each Weyl cone in the FWS renders more exotic gapped phases exhibiting emergent space-time supersymmetry [17] or hosting non-Abelian Majorana modes protected by emergent second Chern numbers [18]. The similar exotic excitonic phases in the FWS with repulsive interactions have also been predicted [19].

In contrast, an interacting phase generated from Weyl semimetal with four or more Weyl points can be either topological or trivial, since each two Weyl cones of the same chirality can be trivially gapped out with e.g. conventional superconducting pairings [20–22].

Albeit having great importance, the FWS has yet to be realized. The very recent success in observing magnetic Weyl semimetals comes closer to realizing FWS in solids [23–25], while challenges still exist due to the complexity of solid materials. Progresses have been also made in simulating topological states in ultracold atoms [26–31]. However, to achieve the FWS in ultracold atoms faces the challenges not only in realizing 3D spin-orbit coupling, which is not yet available, but also in measuring 3D phases [32–38]. Thus realizing the FWS phase is still an outstanding unresolved task. In this work, we solve all the challenges and design a novel lattice scheme to realize the FWS, and propose experimental techniques to detect its 3D band topology based on only 2D measurements. Realization of the FWS can provide a promising platform to explore novel interacting topological states.

The model of realization. We start with the model of 3D Weyl semimetal that we propose to realize via a novel optical Raman lattice scheme. The essential ingredients of realizing the Weyl Hamiltonian include a configuration-tunable 3D optical lattice and periodic Raman potentials which are superposed on and have non-trivial relative symmetries with respect to the lattice, as illustrated in Fig. 1(a-c). The lattice and Raman potentials couple the spin states $|g\uparrow\rangle$ which are two Zeeman-split ground hyperfine levels of atoms. The laser beam ($E_\lambda$) incident along the x direction has polarizations in $y$-$z$ plane, and then is reflected by three mirrors to create orthogonal standing waves [Fig. 1(a)]. Two quarter-wave plates (QWPs) are applied to induce $\pi/2$ phase shift by each between the in-plane ($x$, $y$) and out-of-plane ($z$) polarization components, respectively with the strengths $E_{xy}$ and $E_{xz}$. The electric fields of the $x-y$ plane...
A beam \(E_y\) with \(y\) and \(z\) polarization components (shown in red) is incident along the \(+x\) direction and then reflected and retracted orthogonally through two quarter-wave-plates to form a square lattice in the diagonal directions of \(x - y\) plane: \(x' = (x - y)/\sqrt{2}\) and \(y' = (x + y)/\sqrt{2}\) [the bottom layer of (c)]. A standing-wave beam of slightly higher frequency (shown in blue) is applied and forms the lattice in the \(z\) direction. (b) Two Raman-transitions between the two ground spin states are also induced by the red and blue beams whose frequency difference matches the Zeeman splitting, forming 3D Raman potentials. (c) Illustration of the configurations of the lattice and Raman potentials when \(\delta \omega = \delta \omega_x = \delta \omega_z\) and \(\omega_x = \omega_z\). The two-beam case is treated as a special case with \(\delta \omega = 0\). (d) The Weyl band and phase diagram. The Hamiltonian \(H\) is anti-symmetric with respect to the lattice in \(x'\) \((y')\) direction, but symmetric in other directions. This relative symmetry, as obtained only for the deformed lattice configuration, is essential for realizing the FWS. Note that the \(z = 0\) plane reduces to the 2D quantum anomalous Hall (QAH) model driven by the SO coupling [40, 41]. The Weyl band and phase diagram. The Hamiltonian \(H\) realizes the 3D Weyl semimetal, with the number of Weyl points being tuned by \(m_z\). The Weyl semimetal band can be easily seen from the tight-binding (TB) Hamiltonian, while the results are valid beyond the TB regime. Other than the spin-conserved hopping induced by lattice potential, the Raman potential \(\mathcal{M}(r)\) drives spin-flip hopping along \(x'\) \((y')\) direction, with the hopping coefficient \(t_{\text{SO}}^{m_z}\) as a function of \(m_z\).
Figure 2: Construction of 3D Weyl band topology via 2D measurements. (a) Weyl points and the Berry curvature $\Omega(q)$. Red (blue) spheres located at $k = (0, 0, \pm 0.4k_0)$ are Weyl points of positive (negative) chirality. Red (blue) arrows and slices correspond to positive (negative) $\Omega_z$. (b1) Spin textures of the lower band on different $q_z$ slices (shown from $-k_0/2$ to $k_0/2$). The band-inversion-surface (BIS) is pictured in a series of white rings, where $\langle \sigma_z \rangle = 0$. Inside (outside) the BIS is spin up (down). (b2) – (b4) 2D Band structures on three particular $q_z$ slices: $q_z = 0.5\pi$, $q_z = 0.4\pi$, and $q_z = 0$. On the $q_z = 0.4\pi$ slice, two bands touch at a Weyl point. (c) The $q_z$-integrated 2D spin textures tuned by Zeeman splitting $m_z$, as measurable in real experiments. This effectively maps out the 3D Weyl band topology and Weyl points, as compared to (b1). The parameters: $V_0/E_r = 2$, $V_z/E_r = 4$, $M/E_r = 0.586$, and $m_z/E_r = 0.288$.

$$(t_{SO})_{xy} = \pm (-1)^{\delta_{x',y'} + \delta_{x',y}} t_{SO}$$

and $t_{SO}$ being the amplitude. The staggered sign $(-1)^{\delta_{x',y'} + \delta_{x',y}}$ can be absorbed by a gauge transformation which shifts the Bloch momentum of spin-down state $|q_y\rangle$ by $k_0 = (k_0/\sqrt{2}, k_0/\sqrt{2}, k_0)$ in the three directions [22]. The Bloch Hamiltonian in the quasi-momentum space reads

$$\mathcal{H} = \sum_q \hat{c}_q^\dagger \mathcal{H}(q) \hat{c}_q,$$

where $\hat{c}_q = (\hat{c}_{q,\uparrow}, \hat{c}_{q,\downarrow})$ and

$$\mathcal{H}(q) = \left( m_z - 2t_0 \cos q_{x'} - 2t_0 \cos q_{y'} - 2t_z \cos q_z \right) \sigma_z + 2t_{SO} \sin q_{x'} \sigma_x + 2t_{SO} \sin q_{y'} \sigma_y. \quad (2)$$

Here $q_{x',y'} = \pi k_{x',y'}/k_0$, $q_z = \pi k_z/k_0$ are the dimensionless Bloch momenta, and $t_0 (t_z)$ is the nearest-neighbor hopping coefficient in the $x-y$ plane ($z$ direction). The above 3D Hamiltonian describes a set of 2D QAH layers in $x-y$ plane, each with a fixed $q_z$, stacked in $q_z$ direction. The Weyl points are obtained as the topology of QAH layers changes by varying $q_z$. In particular, the Weyl points correspond to $\mathcal{H}(q_w) = 0$, which requires that $(q_{w,x'}, q_{w,y'}) = (0, 0), (0, \pi), (\pi, 0)$, or $(\pi, \pi)$. Due to reflection symmetry $z \rightarrow -z$, the Weyl points come in pairs at $\pm q_w$ (or none at all). Thus the total number of Weyl points takes even values from 0 to 8. For example, in the TB Hamiltonian, when $m_z = 4t_0$, the FWS with two Weyl points at $q_w = (0, 0, \pm \pi/2)$ is resulted.

The full exact phase diagram for the Hamiltonian (1) is shown numerically with different parameters in Fig. 1(d). The 3D Weyl semimetal phases with $N$ Weyl points are obtained. In particular, the most important FWS phase with $N = 2$ is obtained in a relatively large region, as marked in red-colored area. For the real experiment, the numerical results show that an optimal FWS is obtained when the parameters are taken that $V_0/E_r = 2$, $V_z/E_r = 4$, $M/E_r = 0.586$, $m_z/E_r = 0.288$, where $E_r = (\hbar k_0)^2/2m$ is the recoil energy, and the two Weyl points are located at $q_w = (0, 0, \pm 0.4\pi)$.

Detection. How to detect Weyl points from measuring the 3D Weyl band is challenging but as important as the realization. The standard momentum-space tomography and band mapping are applicable to measure the 1D and 2D band physics, while in measuring 3D phases the band structure of the third dimension is always integrated out and thus not-resolvable. In the following, we solve the challenge and propose both equilibrium and dynamical schemes to map out the Weyl band topology and Weyl points through 2D symmetry-tuned measurements.

Measuring the 3D Weyl band I: equilibrium scheme.– The Weyl semimetal consists of 2D QAH layers in the $x-y$ plane, which change topology across a Weyl point along $q_z$ axis. For a QAH layer and with nonzero Chern number, its 2D bulk band has a band inversion ring in the $q_x - q_y$ plane, which is a 1D version of the band inversion surface (BIS) [23], defined by $h_z(q_x, q_y)|_{\text{fix } q_z} = 0$ and having vanishing spin-polarization along $z$ direction $\langle \sigma_z \rangle |_{q_z} = 0$. Here $\langle \cdot \rangle$ is calculated for the lower band. The $q_z$-sliced 2D spin textures of the lower band are plotted in Fig. 2(b1), where the band inversion rings are clearly obtained. When the 2D QAH layers change topology as the $q_z$ varies [see Fig. 2(b2)], the size of the band inversion ring shrinks to singular points, rendering the Weyl nodes. Therefore, the Weyl points can be detected if the configuration of BIS or the band inversion rings versus $q_z$ can be measured.

The key observation is that the $q_z$-resolved 2D spin textures in $q_x - q_y$ plane can be effectively detected by
We further propose to detect the Weyl points by non-Weyl band topology and the Weyl points in the bulk. Therefore, the virtual slices of the fusiform BIS as shown in Fig. 3(c), the Hamiltonian is suddenly tuned to the target Hamiltonian for FWS phase with small $m_z$. The quench dynamics in momentum space reads \( \langle \sigma_z(q) \rangle(t) = \langle g_q e^{i\omega(t)\mathcal{H}(q)/\hbar} | \sigma_z | e^{-i\omega(t)\mathcal{H}(q')/\hbar} g_q \rangle \), for the short-term dynamics, with damping effects being negligible, the spin process is obtained by \( [42] \)

\[
\langle \sigma_z(q) \rangle(t) = -\langle \sigma_z(q) \rangle^2 - (1 - \langle \sigma_z(q) \rangle^2) \cos(\omega q t), \tag{5}
\]

where \( \langle \sigma_z(q) \rangle \) is the spin-polarization of the lower band of post-quench Hamiltonian and the frequency equals the local band gap, \( \omega(q) = 2|E(q)|/\hbar \). The Weyl points correspond to \( \omega(q_w) = 0 \), and can be precisely determined by projection measurements. First, we project the measurement of \( \langle \sigma_z(q) \rangle \) in the \( q_x - q_y \) plane, and measure the minimal frequency \( \omega_{LB} = \min |\omega(q_w)| \) with every fixed \( (q_x', q_y') \), which determines the Weyl point momentum \( (q_x^w, q_y^w) \) in \( q_x - q_y \) plane. Further, we project the measurement in the \( q_x - q_z \) plane and measure the minimal frequency \( \omega_{LB} = \min |\omega(q_w)| \) with every fixed \( (q_x', q_z) \), determining the Weyl point momentum \( (q_x^w, q_z^w) \). With the two steps we can determine the full Weyl point momentum \( q^w \). This process is illustrated in Fig. 3(b).

Finally we note that the BIS can be also dynamically measured by spin dynamics. The time-averaged spin polarization \( \langle \sigma_z(q) \rangle(t) = \frac{1}{\tau} \int_0^\tau \langle \sigma_z(q) \rangle(t) d\tau = -\langle \sigma_z(q) \rangle^2 \) is negative and approaches zero only in proximity to the BIS \([43]\). Similar to measuring the spin procession frequency, one cannot directly resolve the BIS dynamically in 3D momentum space, but the projection measurement onto 2D spaces can be achieved, with the third dimension being integrated out. Projection to two orthogonal planes, e.g. \( q_x - q_y' \) and \( q_x' - q_z \) planes can determine Weyl point number and momenta in the bulk, as shown in Fig. 3(c).

Figure 3: Precise measurement of Weyl points by quench dynamics. (a) Pre- and post-quench bands and spin states. The Bloch spheres denote the pre- and post-quench spin states of a certain momentum. The spin procession is depicted by a Larmor-type rotation. (b) Colormap of the spin procession frequency, shown on slices of the 3D BZ. The bottom- and sidewalls shows \( \omega_{LB} \) in orthogonal projections onto the \( q_x - q_y' \) plane and \( q_x' - q_z \) plane. Weyl points, being gapless, are captured by two dark spots. (c) Colormap of the averaged spin polarization over certain time. As presented as orthogonal projection view similar to (b), it shows the outline of the BIS as red rings on the slice plot and yellow circles on projection plots.
Conclusion.—We have proposed to realize and detect the FWS based on optical lattice for real experiment. This work already successfully leads to the experimental realization and detection of the FWS [44]. Realization of the FWS opens up a broad avenue to explore with experimental feasibility the exotic interacting topological states in this promising platform.

This work was supported by National Natural Science Foundation of China (11574008, 11761161003, 11825401, and 11921005), National Key R&D Program of China (2016YFA0301604), and Strategic Priority Research Program of Chinese Academy of Science (Grant No. XDB28000000).

* Corresponding author: xiongjunliu@pku.edu.cn

[1] H. Weyl, Proc. Natl. Acad. Sci. U.S.A. 15, 323 (1929).
[2] S.-Y. Xu, I. Belopolski, N. Alidoust, M. Neupane, G. Bian, C. Zhang, R. Sankar, G. Chang, Z. Yuan, C.-C. Lee, et al., Science 349, 613 (2015).
[3] B. Lv, H. Weng, B. Fu, X. Wang, H. Miao, J. Ma, P. Richard, X. Huang, L. Zhao, G. Chen, et al., Phys. Rev. X 5, 031013 (2015).
[4] Xu, S.-Y., et al., Nat. Phys. 11, 748 (2015).
[5] M. Z. Hasan, S.-Y. Xu, I. Belopolski, and S.-M. Huang, Annual Review of Condensed Matter Physics 8, 289 (2017).
[6] L. Lu, Z. Wang, D. Ye, L. Ran, L. Fu, J. D. Joannopoulos, and M. Soljačić, Science 349, 622 (2015).
[7] J. Noh, S. Huang, D. Leykam, Y. Chong, K. P. Chen, and M. C. Rechtsman, Nature Phys. 13, 611 (2017).
[8] Y. Lu, N. Jia, L. Su, C. Owens, G. Juzeliunas, D. I. Schuster, and J. Simon, Phys. Rev. B 99, 020302(R) (2019).
[9] N. Armitage, E. Mele, and A. Vishwanath, Rev. of Mod. Phys. 90, 015001 (2018).
[10] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).
[11] A. A. Burkov and L. Balents, Phys. Rev. Lett. 107, 127205 (2011).
[12] H. B. Nielsen and M. Ninomiya, Nucl. Phys. B 185, 20 (1981).
[13] G. Y. Cho, J. H. Bardarson, Y.-M. Lu, and J. E. Moore, Phys. Rev. B 86, 214514 (2012).
[14] H. Wei, S.-P. Chao, and V. Aji, Phys. Rev. B 89, 014506 (2014).
[15] G. Bednik, A. A. Zyuzin, and A. A. Burkov, Phys. Rev. B 92, 035153 (2015).
[16] T. Zhou, Y. Gao, and Z. D. Wang, Phys. Rev. B 93, 094517 (2016).
[17] S.-K. Jian, Y.-F. Jiang, and H. Yao, Phys. Rev. Lett. 114, 237001 (2015).
[18] C. Chan and X.-J. Liu, Phys. Rev. Leet. 118, 207002 (2017).
[19] Y. Wang and P. Ye, Phys. Rev. B 94, 075115 (2016).
[20] P. Hosur, X. Dai, Z. Fang, and X.-L. Qi, Phys. Rev. B 90, 045130 (2014).
[21] Y. Kim, M. J. Park, and M. J. Gilbert, Phys. Rev. B 93, 214511 (2016).
[22] H. Wang, H. Wang, Y. Chen, J. Luo, Z. Yuan, J. Liu, Y. Wang, S. Jia, X.-J. Liu, J. Wei, and J. Wang, Science Bull. 62, 425 (2017).
[23] D. F. Liu et al., Science 365, 1282 (2019).
[24] N. Morali et al., Science 365, 1286 (2019).
[25] I. Belopolski et al., Science 365, 1278 (2019).
[26] B. Jotzu et al., Experimental realization of the topological Haldane model with ultracold fermions. Nature 515, 237-240 (2014).
[27] Z. Wu et al., Realization of two-dimensional spin-orbit coupling for Bose-Einstein condensates. Science 354, 83-88 (2016).
[28] J.-R. Li et al., A stripe phase with supersolid properties in spin-orbit-coupled Bose-Einstein condensates. Nature 543, 91-94 (2017).
[29] B. Song et al., Observation of symmetry-protected topological band with ultracold fermions. Science advances 4, eaao4748 (2018).
[30] B. Song, C. He, S. Niu, L. Zhang, Z. Ren, X.-J. Liu, and G.-B. Jo, Nature Phys. bf 15, 911 (2019).
[31] N. R. Cooper, J. Dalibard, and I. B. Spielman, Rev. Mod. Phys. 91, 015005 (2019).
[32] Y. Xu, F. Zhang, and C. Zhang, Phys. Rev. Lett. 115, 205504 (2015).
[33] D.-W. Zhang, S.-L. Zhu, and Z. D. Wang, Phys. Rev. A 92, 013632 (2015).
[34] Y. Wang and X.-J. Liu, Predicted scaling behavior of Bloch oscillation in Weyl semimetals. Phys. Rev. A 94, 031603(R) (2016).
[35] W.-Y. He, S. Zhang, and K. T. Law, Realization and detection of Weyl semimetals and the chiral anomaly in cold atomic systems. Phys. Rev. A 94, 013606 (2016).
[36] F. de Juan, A. G. Drusin, T. Morimoto, and J. E. Moore, Nature Comm. 8, 15995 (2017).
[37] D.T. Tran, A. Dauphin, A.G. Drusin, P. Zoller, and N. Goldman, Probing topology by heating: Quantized circular dichroism in ultracold atoms. Science Advances 3, e1701207 (2017).
[38] Y. Xu and Y. Hu, Phys. Rev. B 99, 174309 (2019).
[39] X.-J. Liu, Z.-X. Liu, and M. Cheng, Phys. Rev. Lett. 110, 076401 (2013).
[40] X.-J. Liu, K.-T. Law, and T.-K. Ng, Dirac-, Rashba-, and Weyl-type spin-orbit couplings: Toward experimental realization in ultracold atomic systems. Phys. Rev. A 94, 031603(R) (2016).
[41] B.-Z. Wang et al. Dirac-, Rashba-, and Weyl-type spin-orbit couplings: Toward experimental realization in ultracold atomic systems. Phys. Rev. A 99, 086401 (2014).
[42] B.-Z. Wang et al. Dirac-, Rashba-, and Weyl-type spin-orbit couplings: Toward experimental realization in ultracold atomic systems. Phys. Rev. A 97, 011605 (R) (2018).
[43] See Supplementary Material for more details.
[44] L. Zhang, L. Zhang, S. Niu, and X.-J. Liu, Science Bull. 63, 1835 (2018).
[45] The main results of the present work were completed over one year ago. The experimental study on the present proposal was then initiated, and now the FWS is realized and detected in experiment [44].
[46] C.-R. Yi et al., Manuscript in preparation.
[47] D. A. Steck, "Rubidium 87 d line data" (2001).
Supplementary Material: Realizing and detecting the fundamental Weyl semimetal phase

In this supplementary material we provide the details of deriving the effective Hamiltonian, which is valid for both fermions and bosons (e.g. $^{87}$Rb atoms), and the techniques for measurement.

I. The Model of Realization

A. Laser Setup

As shown in Fig. 1(a) in the main text, two beams forms orthogonal standing wave in the $x-y$ plane, while another beam forms standing wave in the $z$ dimension. The frequencies of the beams are $\omega_1$ for the light $E_{xy}$, $\omega_2 = \omega_1 + \delta \omega$ for the beam $E_{xz}$, and $\omega_3 = \omega_1 + \Delta \omega$ for $E_z$ in the $z$ direction, where $\delta \omega$ matches the Zeeman splitting of the two spin states, $\mu_B g_F B / \hbar$, by a small two-photon detuning $\delta$, and $\Delta \omega$ is in the magnitude of a few MHz. The polarization of the beams are as shown in the Fig.1(a) in the main text. We can conveniently write the light fields as

$$E_{xz} = (\hat{z} E_{xz} e^{ik_0x} + \hat{z} E_{xz} e^{-ik_0y} + \hat{z} E_{xz} e^{-ik_0x}) e^{-i\omega_3 t}$$

$$E_{xy} = (\hat{y} E_{xy} e^{ik_0x} - i\hat{x} E_{xy} e^{-ik_0y} + i\hat{y} E_{xy} e^{-ik_0x}) e^{-i\omega_3 t}$$

$$E_z = \left[ E_z e^{i(k_0z-\omega_2 t)} + E_z e^{i(-k_0z-\omega_2 t)} \right] (\hat{x} + i\hat{y}) / \sqrt{2}$$

where $E_0 = 2E_{xy} = 2E_{xz}$. Here we use $E_{\alpha \beta}$ to represent the laser propagating along $\alpha$-direction with $\beta$-polarization. The wavenumbers are all denoted as $k_0$ because the frequency difference is comparatively small that no observable phase difference is accumulated over the propagation length of the laboratory light path. We further denote $E_{x-y} = E_{xz} + E_{xy}$ for convenience.

B. Lattice Potential and Raman Field

The spin-independent optical potential for typical detuning $\Delta$ is proportional to light intensity, $V_{lat} \propto (E_{x-y}^* E_{x-y} + E_z^* E_z) / \Delta$. For detailed calculation, we sum up coupling induced by the $\sigma^+ / \pi / \sigma^-$ components. Note that the external magnetic field points in $x$ direction, so the $\sigma^+ / \pi / \sigma^-$ components have polarization of $\hat{y} \pm i \hat{z} / 2$ and $\hat{y} \mp i \hat{z} / 2$, respectively. The lattice potentials for $|g_t\rangle$ and $|g_{\perp}\rangle$ are deduced as follow

$$V_{\perp} = \sum_{j=-1/2}^{1/2} \frac{1}{\Delta_j} \left( |\Omega_{j,F,xy}^+(j)|^2 + |\Omega_{j,F,xy}^-(j)|^2 + |\Omega_{j,F,xz}^+(j)|^2 + |\Omega_{j,F,xz}^-(j)|^2 + |\Omega_{j,F,yz}^+(j)|^2 + |\Omega_{j,F,yz}^-(j)|^2 \right)$$

$$= \frac{2}{3} \left( \frac{\alpha_{D_2}^2}{\Delta_{j/2}} + \frac{\alpha_{D_1}^2}{\Delta_{j/2}} \right) (\cos k_0 x \cos k_0 y E_{0}^2 + \cos^2 k_0 y E_{0}^2)$$

$$= -V_0 \cos k_0 x \cos k_0 y - V_z \cos^2 k_0 z,$$

where $\alpha_{D_2}^2 \equiv 2\alpha_{D_1}$ are transition dipole matrix elements can be found in [10]. Similarly, for $|g_t\rangle$ atoms we also have $V_{\parallel} = V_{\perp}$. The key point here is that our lattice potential is deformed and aligned in the diagonal direction. Only in this deformed lattice, the following Raman fields have the symmetry we need to realize Weyl semimetal.

The Raman potentials $M(r)$ are generated by a $\Lambda$-type scheme from bichromatic lights $E_{xy}$ and $E_z$ ($E_{xz}$ does not participate in Raman transitions between the ground states) that couples $|g_{\perp}\rangle$ to $|g_{\parallel}\rangle$, as shown in Fig. 1(b). It can
be explained as an effective Zeeman field. For $^{87}$Rb atoms, the effective Zeeman field has the following form

$$\mathcal{M}(r) = \sum_{j=\frac{1}{2},\frac{3}{2}} \sum_{F} \left( \frac{\Omega_{1}^{(j)} + \Omega_{1}^{(j)} + \Omega_{1}^{(j)}}{\Delta_{j}} + \frac{\Omega_{2}^{(j)} + \Omega_{2}^{(j)} + \Omega_{2}^{(j)}}{\Delta_{j}} \right) \left( \frac{\alpha_{\Delta z}}{12} \frac{1}{\Delta_{3/2}} - \frac{\alpha_{\Delta z}}{6} \frac{1}{\Delta_{1/2}} \right) \left( \frac{E_{xy}^{r} E_{yx}^{r} + E_{zx}^{r} E_{zx}^{r}}{\sqrt{2}} \right)$$

(S3)

$$= M_0 \cos k_0 z (\sin k_0 x \sigma_x + \sin k_0 y \sigma_y).$$

C. Weyl Hamiltonian

Combining the results of Raman field $\mathcal{M}(r)$ and lattice potential $\mathcal{V}_{\text{latt}}(r)$, we arrive at the target Hamiltonian

$$\mathcal{H} = \left[ \frac{p^2}{2m} + \mathcal{V}_{\text{latt}}(r) \right] \| + \mathcal{M}_x(r) \sigma_x + \mathcal{M}_y(r) \sigma_y + m_z \sigma_z.$$  

(S4)

It is apparent that the lattice potential in the $x-y$ plane is diagonally aligned. To align the lattice with the coordinate axes, we rotate the axis in the $x-y$ plane by $\pi/4$ such that $x' = (x-y)/\sqrt{2}$ and $y' = (x+y)/\sqrt{2}$. Under this rotation in the real space, the Hamiltonian can be write in the square lattice as

$$\mathcal{H} = \left( \frac{p^2}{2m} - \frac{V_0}{2} \cos^2 k_0 x' - \frac{V_0}{2} \cos^2 k_0 y' - V_z \cos^2 k_0 z \right) \| + m_z \sigma_z$$

$$+ \sqrt{2}M_0 \cos k_0 z \left[ \sin(k_0' x') \cos(k_0' y') \sigma_x + \cos(k_0' x') \sin(k_0' y') \sigma_y \right].$$

(S5)

Here we have $k_0' = k_0/\sqrt{2}$ after rotation.

To get a more intuitive understanding of our Hamiltonian, we take it to the tight-binding(TB) picture. Under the deep lattice limit, the atoms are positioned at the bottom of the lattice sites, while the spin-reserved (spin-flipping) hopping terms are decided by the inter-site overlap of Wannier wavefunctions (plus Raman potential), respectively. We observe that the Raman potentials are in staggered superposition over the lattice cells. Therefore, a staggered gauge transformation $U = e^{i(k_0' x' + k_0' y' + k_0 z)} |q_1\rangle \langle q_1|$ can be applied on the spin-down state as was performed in 2D SOC system [40]. Then the tight-binding Hamiltonian in the momentum space can be written as

$$H(q) = \hbar(q) \cdot \sigma$$

$$= (m_z - 2t_0 \cos q_x - 2t_0 \cos q_y - 2t_z \cos q_z) \sigma_z + 2t_{\text{SO}} \sin q_x \sigma_x + 2t_{\text{SO}} \sin q_y \sigma_y.$$  

(S6)

The band-inversion-surface(BIS) satisfies the equation $h_z(q) = 0$. We can see that the Weyl points should be located at the intersections of the BIS and one of these four lines along the $q_z$ direction: $(q_x', q_y') = (0, 0), (0, \pi), (\pi, 0), (\pi, \pi)$. On each line there must be a pair of Weyl points of opposite $q_z$ and opposite Weyl charge (or none at all), due to reflection symmetry of the BIS.

Here we are especially interested in the system that have only two Weyl points, which can be realized in the conditions $|m_z| > 2t_z$ or $-2t_0 < 4t_0 - |m_z| < 2t_z$. As an example, under these chosen parameters $V_0 = 2E_r$, $V_z = 4E_r$, $M = 0.586E_r$, we can tune $m_z = 0.288E_r$ so that $N = 2$, the only two Weyl points are located at $q = (0, 0, \pm 0.4\pi)$.

E. Nodal-line Semimetal Hamiltonian

For overall blue detuned cases, where $(\frac{2}{\Delta_{3/2}} + \frac{1}{\Delta_{1/2}})$ is positive, $V_0$ and $V_z$ becomes negative so that the peaks and valleys of the potential are switched. However, the Raman field remains the same. As the result, the spin-flipped hopping vanish on the in-plane nearest neighbor couplings, but instead appears on the second-nearest neighbor sites in the adjacent plane.

To study the properties of a blue-detuned Hamiltonian, we consider its TB limit, Which differs from the red-detuned case only by the off-plane spin-flipped hopping terms. Following the same staggering transformation, we arrive at the momentum space Hamiltonian

$$H(q) = (m_z - 2t_0 \cos q_x - 2t_0 \cos q_y - 2t_z \cos q_z) \sigma_z + 4t_{\text{SO}} \sin q_x \sigma_x + 4t_{\text{SO}} \sin q_y \sigma_y.$$  

(S7)
It is readily seen that the BIS remains basically the same as the red-detuned case, and while the Weyl points are still located at the intersection points between the BIS and \((q_{x'}, q_{y'}) = (0, 0), (0, \pi), (\pi, 0),\) and \((\pi, \pi)\) lines, the intersection line(s) of the BIS and the \(q_x = 0\) and \(q_z = \pi\) plane are the new gapless nodal line(s).

In particular, the nodal line(s) appear alongside the Weyl points in the blue-detuned case, as shown in Fig. 1(d4) in the main text. In particular, in the TB regime, the number of nodal lines \(N_L\) and the number of Weyl points \(N_P\) should follow the simple relation: \(2 - N_L = |2 - N_P^e|\), in which \(N_L = N_P = 0\) is the trivial phase.

\section{Measuring the 3D Weyl band: Virtual Slicing Technique}

There is an equivalent method to scan the \(q_z\) for BIS measurement: the Virtual Slicing Technique. While a 3D ToF imaging is technically challenging, it is easy to perform a 2D ToF imaging of spin polarization with \(q_z\) projected out: \(\langle \sigma_z \rangle = \frac{1}{2\pi} \int_0^{2\pi} \langle \sigma_z \rangle dq_z\). We prove that scanning \(q_z\) in \(\langle \sigma_z \rangle\) can be mimicked by tuning \(m_z\) in \(\langle \sigma_z \rangle\). First, \(\text{sgn}(\langle \sigma_z \rangle) = \text{sgn}(h_z(q)) = \text{sgn}(m_z - 2t_0 \cos q_{x'} - 2t_0 \cos q_{y'} - 2t_z \cos q_z)\). Therefore, \(\text{sgn}(\langle \sigma_z \rangle) = \text{sgn}(m_z - 2t_0 \cos q_{x'} - 2t_0 \cos q_{y'})\). Second, tuning \(m_z\) is equivalent to scanning \(q_z\), \(\langle \sigma_z \rangle\) changes from \(\langle \sigma_z \rangle_{\theta=0} = \cos q_z\) to \(\langle \sigma_z \rangle_{\theta=\pi} = -\cos q_z\). This also be understood as scanning a virtual momentum axis \(q_m = \pm \frac{\pi}{t_0} \arccos \left(\frac{\Delta m_z}{2t_z}\right)\). Finally we arrive at

\[\text{sgn} \left(\langle \sigma_z \rangle\right) = \text{sgn} \left(\langle \sigma_z \rangle_{\theta=0} \right)\].

(S8)

Therefore, the virtual slices of the BIS can be obtained by simply varying \(m_z\). Compared to the actual atom slices, the BIS on these virtual slices are thicker because the cross-over from positive polarization to negative polarization is smoothed out from the \(q_z\) integral.

\section{Measuring the 3D Weyl band: Quench Dynamics}

\subsection{A. Lindblad Master Equation and Spin Oscillation}

To study the dynamic evolution of a given initial quantum state, we use a reduced model of the Lindblad Master Equation on the tight-binding spin state of a given momentum

\[\dot{\rho}(t) = -i[H, \rho(t)] + \gamma \left[ L_+ \rho(t)L_+ - \frac{1}{2} \{ L_+^\dagger L_-, \rho(t) \} \right],\]

(S9)

where we take the TB Hamiltonian in Eq. \(H(q) = h(q) \cdot \sigma = (m_z - 2t_0 \cos q_{x'} - 2t_0 \cos q_{y'} - 2t_z \cos q_z)\sigma_z + 2t_{SO} \sigma_x + 2t_{SO} \sigma_y\) for a given \(q\). Its corresponding eigenstates are \(|1\rangle = \sin \frac{\theta}{2} |g_z\rangle - \cos \frac{\theta}{2} e^{i\phi} |g_r\rangle\) for the lower band eigenstate, and \(|2\rangle = \cos \frac{\theta}{2} |g_r\rangle + \sin \frac{\theta}{2} e^{i\phi} |g_z\rangle\) for the upper band eigenstate. Accordingly, we denote the new ground-state average \(\langle 1|\sigma|1\rangle = \langle \sigma \rangle_g\). In addition, \(L_- = |1\rangle\langle 2|\), and the pre-quench state \(\rho(0) = |g_z\rangle\langle g_z|\).

The solution to the master equation, in the form of Bloch vector \(a(t) = \langle \sigma \rangle(t)\) (as shown in Fig. S1(a1)), reads

\[a(t) = R_\phi(\theta + \pi) R_\phi(-\theta) a'(t),\]

(S10)

where \(R_k(\theta)\) denotes the elemental rotation matrix around \(k\)-axis, \(\theta = \arccos(\langle \sigma_z \rangle_g)\), \(\phi = \arctan(\langle \sigma_x \rangle_g / \langle \sigma_y \rangle_g)\), and \(a'(t) = (-\sin \theta e^{-\gamma t/2} \cos \omega t, -\sin \theta e^{-\gamma t/2} \sin \omega t, (1 - \cos \theta) e^{-\gamma t} - 1)^T\) where \(\omega = 2|h(q)|\). Finally we arrive at the time-evolution of the spin polarization:

\[\langle \sigma_z \rangle(t) = -\left(1 - \langle \sigma_z \rangle_g\right) e^{-\gamma t/2} \cos \omega t + \langle \sigma_z \rangle_g \left(1 - (\langle \sigma_z \rangle_g + 1) e^{-\gamma t}\right).\]

(S11)

It is in the form of a damped oscillation overlaying an exponential base function, shown as the blue curve in Fig. S1(a2). The quality factor of the oscillation \(Q = \omega / \gamma\).

To average out the effect of the oscillation from the base function, we define time-averaged spin polarization as:

\[\langle \langle \sigma_z \rangle(t) \rangle = \frac{1}{t} \int_0^t \langle \sigma_z \rangle(\tau) d\tau = \langle \sigma_z \rangle_g - \frac{1}{t} \left[ \frac{2(1 - \langle \sigma_z \rangle_g)(-\gamma \cos \omega t + 2\omega \sin \omega t) e^{-\frac{2\gamma t}{\gamma}}}{\gamma^2 + 4\omega^2} + \frac{\langle \sigma_z \rangle_g(1 + \langle \sigma_z \rangle_g)(1 - e^{-\gamma t})}{\gamma} \right],\]

(S12)
which damps away much more quickly (shown as the orange/red curve in Fig. S1(a2)), and at $Q \to \infty$, converges to

$$\langle \sigma_z \rangle(t) = \langle \sigma_z \rangle_g - \frac{1}{\gamma t} \langle \sigma_z \rangle_g (1 + \langle \sigma_z \rangle_g) (1 - e^{-\gamma t}).$$  \hspace{1cm} (S13)

It is evident that the short-time behavior of $\langle \sigma_z \rangle(t)$ ($\frac{16}{\omega} < t < 0.1 \frac{Q}{\omega}$) differs from long-time behavior ($t > 10 \frac{Q}{\omega}$). In the short- and long- time limit we get $\langle \sigma_z \rangle(0) = -\langle \sigma_z \rangle^2_g$ and $\langle \sigma_z \rangle(\infty) = \langle \sigma_z \rangle_g$, respectively. As a result, the band inversion surface (BIS) is stressed out under projection in $\langle \sigma_z \rangle(0)$ compared to the long-time limit because in the former case spin-polarization takes negative value over the entire Brillouin zone. In Fig. S1(b1-b3) we illustrate how the spin-polarization and projected-spin-polarization change with respect to time evolution in the high-$Q$ limit. This is the advantage of the quench method: in the static spin polarization measurement, the positive and negative polarizations cancel out each other after projection, covering up the shape of the BIS; while in the long-time behavior of $\langle \sigma_z \rangle(t)$, the positive polarization only exist near the BIS, so the outline of the BIS is preserved after projection, as shown in Fig. S1(b3). From the side- and bottom- projection images, we can recreate the outline of the BIS in 3D Brillouin zone.

**B. LB Energy Spectroscopy**

In comparison to the static measurements, the quenching method is clearly more informative as it utilizes the time domain. Thus it offers higher resolution on the energy axis, and provides essential information on the structure of the BIS and location of the Weyl points with the projected 2D ToF image alone. One of the ways one can make use of
Figure S2: (a) Frequency spectrum of certain points in the projected $k_x' - k_z$ plane at $Q_{max} = 50$. Each spectrum curve has two peaks, where the left (right) peak corresponds to the lower (upper) bound frequency along the projection line. (b) Colormap of the Larmor frequencies. The bottom- and side-walls shows $\omega_{LB}$ in orthogonal projection. Weyl points, being gapless, are presented as two dark spots. The white dots on the side projection correspond to the spectra curves in (a). As we move away from the projection of Weyl points in the order of $P_1 \rightarrow P_6$, the signal-strengths of the peaks of the spectra curves gradually lower while their frequencies increase.

the real-time evolution is by marking out the lower-bound frequency of Larmor frequencies on all the points along a projection line - we call this method the lower-bound (LB) energy projection spectroscopy - which roots in the linearity of Fourier transformation.

In Fig. S2(b), the frequency projection images of the 3D Larmor frequency plot are shown as orthographic projections on the side- and bottom-walls, or the $q_{x'} - q_z$ and $q_{x'} - q_{y'}$ plane, respectively. Fig. S2(b) demonstrates how to obtain $\omega_{LB}$ using the $q_{y'}$-projected imaging in the $q_{x'} - q_z$ plane as example. First, one can obtain an amplitude-frequency ($\tilde{A} - \omega$) curve for every point on the $q_{x'} - q_z$ plane by performing a Fourier transformation on the (projected) spin polarization oscillation data (here we introduce damping in the system so that the highest Q is $\sim 50$).

\[ \tilde{A}(\omega) = \mathcal{F} \left[ \frac{1}{2\pi} \int_0^{2\pi} \langle \sigma_z(t) \rangle \, dq_{y'} \right] = \frac{1}{2\pi} \int_0^{2\pi} \mathcal{F} \left[ \langle \sigma_z(t) \rangle \right] \, dq_{y'}. \]  

What we get essentially is a summation of all the frequency-response curves along the $q_{y'}$ dimension, which results in peaks at the lowest and the highest frequencies along the integrated line. This is due to the fact that projection doesn’t change frequency, but instead highlights the lowest and the highest frequency responses because the density of states at these frequencies are infinity (in theory, the two peaks of each frequency spectra curve should be infinitely tall and narrow, but the damping in the oscillation widens the peak-width). From the LB projection plots, we can straightforwardly mark out the position of each individual Weyl points, as the energy difference vanishes. Because the bands are essentially smooth, we can also infer the linear dispersion around the Weyl point from the linearity of the projected LB energy difference.

Points in some areas (separated by white lines in Fig. S2(b)) on the corners of LB frequency projection plots may have uncertain $\omega_{LB}$ at the presence of noise because their LB peak signal is not obvious - such as the $P_6$ curve in Fig. S2(a) - rendering these areas unresolvable. However, by cross-examining with the shape of the BIS in Fig. S1(b), we know that these low signal-to-noise-ratio areas are far from the BIS, and thus do not contain any Weyl points.

Note that compared to the LB frequency projection, the maximal spin polarization projection images are deduced more straightforwardly. Unlike frequency which is remained after projection, projection averages out the spin polarization.