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Floquet multi-Weyl points in crossing-nodal-line semimetals

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Weyl points with monopole charge ± 1 have been extensively studied; however, real materials of multi-Weyl points, whose monopole charges are higher than 1, have yet to be found. In this Rapid Communication, we show that nodal-line semimetals with nontrivial line connectivity provide natural platforms for realizing Floquet multi-Weyl points. In particular, we show that driving crossing nodal lines by circularly polarized light generates double-Weyl points. Furthermore, we show that monopole combination and annihilation can be observed in crossing-nodal-line semimetals and nodal-chain semimetals. These proposals can be experimentally verified in pump-probe angle-resolved photoemission spectroscopy.

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Introduction. Stimulated by extensive studies on topological insulators [1–3], it has now been realized that many metals also have topological characterizations [3–5]. In these topological semimetals, the valence band and conduction band touch at certain **k**-space manifolds. When the band-touching manifolds consist of isolated points, the materials are nodal-point semimetals, Dirac semimetals [6–15], and Weyl semimetals (WSMs) [16–39] being the most well-known examples; when the band-touching manifolds are one-dimensional lines, the systems are nodal-line semimetals (NLSMs) [40–77].

In WSMs, the Weyl points are the sources or sinks of Berry magnetic field, namely, they are the Berry monopole charges. The total number of monopole charges in the Brillouin zone must be zero, which has been formulated decades ago as a no-go theorem by Nielsen and Ninomiya [78]. Usually, a Weyl point has a linear dispersion in all three spatial directions, with a low-energy Hamiltonian $H(\mathbf{q}) = \sum_{i,j=x,y,z} v_{ij} q_i \tau_j$, where $\tau_{x,y,z}$ are the Pauli matrices. The monopole charge is just $C = \mathrm{sgn}[\det(v_{ij})] = \pm 1$. Interestingly, multi-Weyl points with monopole charge higher than one are also possible. The simplest cases are the double-Weyl points with $C = \pm 2$ [79–81], which have novel physical consequences [82–87]. So far, the double-Weyl points have not been experimentally realized in solid-state materials. Considering the widespread interests in WSMs, it is highly interesting to find material realizations of multi-Weyl points. The combination of several Weyl points into a multi-Weyl point, and the annihilation of several Weyl points are even more interesting to investigate; nevertheless, it is challenging to do so because of the limited tunability in the samples.

Over the past few years, periodic driving has been used as a powerful method to alter the topology of static systems, and more remarkably, to create new topological phases without analog in static systems [88–109]. Recently, there are a few theoretical proposals for Floquet topological semimetals [110–121]; in particular, it has been suggested that under a circularly polarized light (CPL), NLSMs will be driven to Floquet WSMs with highly tunable Weyl points [116–118,122]. In these studies, only the simplest nodal lines are considered. The present work is stimulated by recent proposals of novel nodal lines with nontrivial connectivity, including crossing nodal lines [54,55,123,124] (probably the most interesting ones are the nodal chains [58,125,126]), nodal links [127–130], and nodal knots [131]. In this Rapid Communication, we show that crossing nodal lines (including nodal chains) are natural platforms for the realizations of Floquet multi-Weyl points and the combinations (annihilations) of Weyl points. In particular, a two-nodal-line crossing point can be driven to a double-Weyl point, and tuning the direction of incident lasers can induce monopole combination transitions. Considering the abundant material candidates for crossing nodal lines [52–58,123], we believe that this proposal can be experimentally verified in the near future.

Double-Weyl points from type-I crossing. For simplicity, we focus on NLSMs with negligible spin-orbit coupling [54,55]. We distinguish two types of nodal-line crossing, illustrated in Figs. 1(a) and 1(b), as type-I and type-II crossing, respectively. The type-II crossing is the basic building block of nodal chains. In this section, we focus on the type-I crossing. Our starting point is the following Bloch Hamiltonian ($\hbar = c = k_B = 1$):

$$H(\mathbf{k}) = (m - Bk^2)\tau_x + \lambda k_y k_z \tau_z + \epsilon_0(\mathbf{k})\tau_0, \tag{1}$$

where $\tau_{x,y,z}$ are Pauli matrices in orbital space and τ_0 is the identity matrix, m is a positive constant with the dimension of energy, B and λ are positive constants with the dimension of inverse energy, and $k^2 = k_x^2 + k_y^2 + k_z^2$. As the diagonal term $\epsilon_0(\mathbf{k})$ does not affect the main physics, we will neglect it hereafter. The energy spectra of this Hamiltonian read

$$E_{\pm,\mathbf{k}} = \pm\sqrt{(m - Bk^2)^2 + \lambda^2 k_y^2 k_z^2}. \tag{2}$$

It is readily found that there are two nodal lines: one is located in the $k_z = 0$ plane and determined by the equation $k_x^2 + k_y^2 = m/B$, while the other one is located in the $k_y = 0$ plane and determined by the equation $k_x^2 + k_z^2 = m/B$. The two nodal lines cross at $\mathbf{K}_\pm = \pm(\sqrt{m/B},0,0)$, which gives the type-I crossing illustrated in Fig. 1(a). The crossing points are protected by the mirror symmetry: $\mathcal{M}_z H(k_x,k_y,k_z)\mathcal{M}_z^{-1} = H(k_x,k_y,-k_z)$ and $\mathcal{M}_y H(k_x,k_y,k_z)\mathcal{M}_y^{-1} = H(k_x,-k_y,k_z)$ with $\mathcal{M}_z = \mathcal{M}_y = \tau_x$.

We study the effects of a CPL. Let us consider a CPL incident in the direction $\mathbf{n} = (\cos\phi\ \sin\theta, \sin\phi\ \sin\theta, \cos\theta)$, where θ and ϕ are the polar and azimuthal angle in the spherical coordinate system, respectively. The vector potential of the light is $\mathbf{A}(t) = A_0[\cos(\omega t)\mathbf{e}_1 + \eta\ \sin(\omega t)\mathbf{e}_2]$,

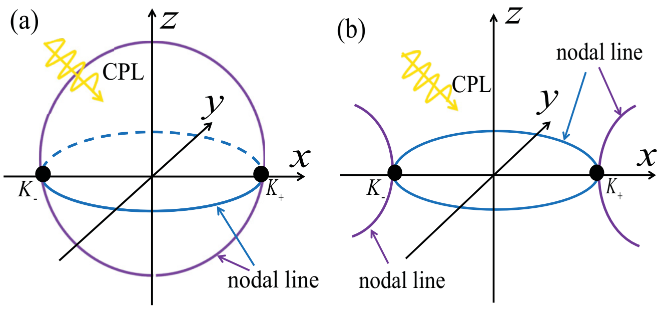

FIG. 1. Two types of nodal-line crossing. (a) Type-I crossing: two nodal lines are located on the same side of the tangential plane (the $k_x = \pm|\mathbf{K}_+|$ planes) near their crossing points. (b) Type-II crossing: two nodal lines are located on the opposite side of the tangential plane near their crossing points.

with $\eta = \pm 1$ corresponding to the right-handed and left-handed CPL, respectively. Here, $\mathbf{e}_1 = (\sin\phi, -\cos\phi, 0)$ and $\mathbf{e}_2 = (\cos\phi\,\cos\theta, \sin\phi\,\cos\theta, -\sin\theta)$ are two unit vectors perpendicular to $\mathbf{n}$, satisfying $\mathbf{e}_1 \cdot \mathbf{e}_2 = 0$.

Following the standard approach, the electromagnetic coupling is given by $H(\mathbf{k}) \to H[\mathbf{k} + e\mathbf{A}(t)]$. Since the full Hamiltonian is time-periodic, it can be expanded as $H(t,\mathbf{k}) = \sum_n H_n(\mathbf{k})e^{in\omega t}$ with

$$\begin{aligned} H_0(\mathbf{k}) &= [\tilde{m} - Bk^2]\tau_x + (\lambda k_y k_z - 2D_1)\tau_z, \\ H_{\pm 1}(\mathbf{k}) &= -BeA_0[(\sin\phi k_x - \cos\phi k_y) \\ &\quad \mp i\eta(\cos\phi\,\cos\theta k_x + \sin\phi\,\cos\theta k_y - \sin\theta k_z)]\tau_x \\ &\quad - \lambda e A_0[\cos\phi k_z \pm i\eta(\sin\phi\,\cos\theta k_z - \sin\theta k_y)]\tau_z/2, \\ H_{\pm 2}(\mathbf{k}) &= (D_1 \mp i\eta D_2)\tau_z, \end{aligned} \tag{3}$$

and $H_n = 0$ for $|n| > 2$; $\tilde{m} = m - Be^2A_0^2$, $D_1 = \lambda e^2 A_0^2 \sin\phi\,\cos\theta\,\sin\theta/4$, $D_2 = \lambda e^2 A_0^2 \cos\phi\,\sin\theta/4$. We focus on the off-resonance regimes, and the system is well described by an effective time-independent Hamiltonian, which reads [89,132]

$$\begin{aligned} H_{\text{eff}}(\mathbf{k}) &= H_0 + \sum_{n\geqslant 1} \frac{[H_{+n}, H_{-n}]}{n\omega} + \mathcal{O}\left(\frac{1}{\omega^2}\right) \\ &= (\tilde{m} - Bk^2)\tau_x + (\lambda k_y k_z - 2D_1)\tau_z \\ &\quad + \gamma\eta\big[(\cos\theta k_z - \sin\phi\,\sin\theta k_y)k_x \\ &\quad + \cos\phi\,\sin\theta\big(k_y^2 - k_z^2\big)\big]\tau_y + \cdots, \end{aligned} \tag{4}$$

where $\gamma = -2B\lambda e^2 A_0^2/\omega$. Consequently, the energy spectra of H_{eff} are

$$\begin{aligned} E_\pm(\mathbf{k}) = \pm\big\{&(\tilde{m} - Bk^2)^2 + (\lambda k_y k_z - 2D_1)^2 + \gamma^2\big[(\cos\theta k_z \\ &- \sin\phi\,\sin\theta k_y)k_x + \cos\phi\,\sin\theta\big(k_y^2 - k_z^2\big)\big]^2\big\}^{1/2}. \end{aligned} \tag{5}$$

For a general incident direction other than $\phi = 0$, π, and $\theta = 0$, $\pi/2$, π, it is readily found from Eq. (5) that there are four Floquet Weyl points. Since $eA_0 \ll \sqrt{m/B}$ under experimental conditions, the D_1 term can be neglected because it only induces a small and trivial change to the positions of the Weyl points. Discarding the D_1 term, it is straightforward to determine the positions of the Weyl points, which are at

$$\begin{aligned} \mathbf{Q}_1 &= -\mathbf{Q}_2 = \frac{\sqrt{\tilde{m}/B}}{\sqrt{(\cos\phi\,\sin\theta)^2 + \cos^2\theta}}(\cos\phi\,\sin\theta, 0, \cos\theta), \\ \mathbf{Q}_3 &= -\mathbf{Q}_4 = \sqrt{\tilde{m}/B}(\cos\phi, \sin\phi, 0). \end{aligned} \tag{6}$$

We can expand H_{eff} around these points as $H_{\alpha=1,2,3,4}(\mathbf{q}) = \sum_{ij} v_{\alpha,ij} q_i \tau_j$ with $\mathbf{q} = \mathbf{k} - \mathbf{Q}_\alpha$ referring to the momentum relative to the gapless points. The monopole charge of the Weyl point at $\mathbf{Q}_\alpha$ is simply $C_\alpha = \text{sgn}[\det(v_{\alpha,ij})]$. A straightforward calculation gives

$$C_1 = -C_2 = C_3 = -C_4 = \eta. \tag{7}$$

The number of monopoles is equal to the number of antimonopoles, automatically satisfying the Nielsen-Ninomiya theorem [78]. From Eqs. (6) and (7), it is readily seen that with the variation of (θ,ϕ) and the handedness of the light, both the positions and the monopole charges are tunable. Most interestingly, when the direction $(\phi,\theta) = (0,\pi/2)$ or $(\pi,\pi/2)$ is reached, we can observe the combination of two Weyl points with the same monopole charge to form a double-Weyl point. To see this more clearly, notice that when the light comes in the x direction, i.e., $\phi = 0$, $\theta = \pi/2$, H_{eff} in Eq. (4) reduces to the form of

$$H_{\text{eff}}(\mathbf{k}) = (\tilde{m} - Bk^2)\tau_x + \lambda k_y k_z \tau_z + \eta\gamma\big(k_y^2 - k_z^2\big)\tau_y, \tag{8}$$

which gives two gapless points at $\mathbf{Q}_\pm = \pm(\sqrt{\tilde{m}/B}, 0, 0)$. A calculation of the Berry-flux number passing through the surface enclosing $\mathbf{Q}_+$ or $\mathbf{Q}_-$ yields the monopole charges, which are

$$C_\pm = \pm 2\eta, \tag{9}$$

i.e., they are double-Weyl points. A picture illustration of the motion and combination of Weyl points, as (θ,ϕ) is tuned, is shown in Fig. 2(a).

Before closing this section, we briefly discuss crossing nodal lines with cubic symmetry, keeping in mind that several material candidates of NLSM are found to belong to this class [55,56,123]. The cubic symmetry guarantees the existence of three nodal lines located in mutually orthogonal planes, and the nodal lines are mutually crossing. Since the crossing is still the type I, the physics of Floquet double-Weyl points and monopole combination is similar to that of Eq. (1) (see Supplemental Material for details [133]).

Monopole annihilation from type-II crossing. Now we turn to the type-II crossing [see Fig. 1(b)], which serves as the key building block of the nodal chain [58,125,126]. The local Hamiltonian near the type-II crossing point can be captured by the following continuum Hamiltonian:

$$H(\mathbf{k}) = \big[m - B\big(k_x^2 + k_y^2\big) + Bk_z^2\big]\tau_x + \lambda k_y k_z \tau_z, \tag{10}$$

whose energy spectra are

$$E_{\pm,\mathbf{k}} = \pm\sqrt{\big[m - B\big(k_x^2 + k_y^2\big) + Bk_z^2\big]^2 + (\lambda k_y k_z)^2}. \tag{11}$$

Thus, there is a nodal ring at $k_z = 0$, $k_x^2 + k_y^2 = m/B$, as well as two open nodal lines of hyperbolic shape at $k_y = 0$, $k_x^2 - k_z^2 = m/B$. The three nodal lines touch at two points $\mathbf{K}_\pm = \pm(\sqrt{m/B}, 0, 0)$, which gives the type-II crossing shown in Fig. 1(b).

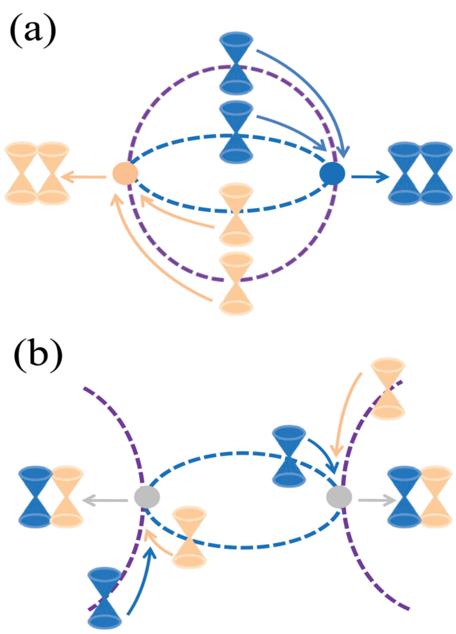

FIG. 2. Illustration of the combination and annihilation process of Weyl points. The different colors of the Weyl cones stand for different monopole charges. The incident angle of the light follows a path in a great circle passing $(\phi,\theta) = (\pi/2,\pi/4)$ and $(0,\pi/2)$. (a) For the type-I crossing, two Weyl points with the same monopole charge come close and form a double-Weyl point. (b) For the type-II crossing, two Weyl points with opposite monopole charge come close and form a critical gapless point. The arrows indicate how the Weyl points move with decreasing ϕ.

Again we consider an incident light described by $\mathbf{A}(t) = A_0[\cos(\omega t)\mathbf{e}_1 + \eta\sin(\omega t)\mathbf{e}_2]$ and follow the procedures of the previous section; we find that the effective Floquet Hamiltonian takes the form of [133]

$$\begin{aligned}H_{\text{eff}}(\mathbf{k}) = {}&\big[m(\theta) - B\big(k_x^2 + k_y^2\big) + Bk_z^2\big]\tau_x + (\lambda k_y k_z - 2D_1)\tau_z\\ &+ \gamma\eta\big[D_3 + (\cos\theta k_z - \sin\phi\,\sin\theta k_y)k_x\\ &+ \cos\phi\,\sin\theta\big(k_y^2 + k_z^2\big)\big]\tau_y,\end{aligned} \tag{12}$$

where $m(\theta) = m - Be^2A_0^2\cos^2\theta$, and $D_3 = -D_2Be^2A_0^2\sin^2\theta/(\gamma\omega)$. The D_3 term is fourth order in eA_0, which is small, thus we first neglect it.

For a general incident angle, similar to the type-I case, the effect of the D_1 term can be neglected. It is straightforward to find the four Weyl points at

$$\begin{aligned}\mathbf{Q}_1' = -\mathbf{Q}_2' &= \frac{\sqrt{m(\theta)/B}}{\sqrt{(\cos\phi\,\sin\theta)^2 - \cos^2\theta}}\\ &\quad\times(-\cos\phi\,\sin\theta, 0, \cos\theta),\\ \mathbf{Q}_3' = -\mathbf{Q}_4' &= \sqrt{m(\theta)/B}(\cos\phi, \sin\phi, 0).\end{aligned} \tag{13}$$

The corresponding monopole charges are found to be

$$\begin{aligned}C_1' &= -C_2' = \eta,\\ C_3' &= -C_4' = \eta.\end{aligned} \tag{14}$$

Thus, both the positions and the monopole charges of the Weyl points are highly tunable. When the incident direction of the light is tuned to the x direction, i.e., $\phi = 0$ and $\theta = \pi/2$, it is readily seen from Eq. (13) that $\mathbf{Q}_1'$ and $\mathbf{Q}_4'$ will overlap, similarly for $\mathbf{Q}_2'$ and $\mathbf{Q}_3'$. Equation (14) tells us that their monopole charges are opposite, thus the annihilation of two Weyl points with opposite monopole charge will occur, and a gapless point with $C = 0$ is found as the remnant of annihilation. To be explicit, let us write down H_{eff} for $\phi = 0$ and $\theta = \pi/2$:

$$\begin{aligned}H_{\text{eff}}(\mathbf{k}) = {}&\big[m - B\big(k_x^2 + k_y^2\big) + Bk_z^2\big]\tau_x + \lambda k_y k_z\tau_z\\ &+ \gamma\eta\big(k_y^2 + k_z^2\big)\tau_y.\end{aligned} \tag{15}$$

There are only two gapless points, namely, $\mathbf{K}_\pm$. It is readily found that the monopole charges of $\mathbf{K}_\pm$ are both zero. In fact, the sign of the coefficient of τ_z is the same for all $\mathbf{k}$, preventing a nonzero winding of the pseudospin vector around the origin, thus the monopole charge has to vanish.

Thus, monopole annihilation can be observed using nodal lines with type-II crossing [Fig. 2(b)]. Since $\mathbf{K}_\pm$ have vanishing monopole charge, they are unstable, i.e., they can be gapped out by a perturbation of the form $\Delta\tau_z$ (Δ denotes a constant).

Now we come back to the effects of the D_3 term. With the D_3 term, we find that the energy spectra have a small gap $2|\gamma D_3|$ at $\mathbf{K}_\pm$ when the light comes in the x direction (i.e., a Floquet insulator). Therefore, when the direction of light is tuned away from the x direction to other directions, the system undergoes an insulator-WSM transition at a certain incident angle, namely, pairs of Weyl points with opposite monopole charges are created from the Floquet insulators.

Surface-state evolution. A key character of Weyl semimetals is the surface Fermi arcs. With the creation of multi-Weyl points, multiple Fermi arcs are naturally expected. We now check it by explicit calculations. Let us focus on the type-I crossing (the similar analysis of type-II crossing is given in the Supplemental Material). We consider that the system occupies the $z > 0$ region. The energy dispersion and the wave functions of the surface states can be determined by solving the eigenvalue problem $H_{\text{eff}}(k_x,k_y,-i\partial_z)\Psi(x,y,z) = E(k_x,k_y)\Psi(x,y,z)$, under the boundary conditions $\Psi(z = 0) = 0$ and $\Psi(z \to +\infty) = 0$. For simplicity, we neglect the D_1 term at this stage, and take the driving-induced τ_y term as a perturbation (this is justified as both D_1 and γ are small), namely, $H_{\text{eff}} \simeq H_0 + \Delta H$ with

$$\begin{aligned}H_0(\mathbf{k}) &= (\tilde{m} - Bk^2)\tau_x + \lambda k_y k_z\tau_z,\\ \Delta H(\mathbf{k}) &= \gamma\eta\big[(\cos\theta k_z - \sin\phi\,\sin\theta k_y)k_x\\ &\quad + \cos\phi\,\sin\theta\big(k_y^2 - k_z^2\big)\big]\tau_y.\end{aligned} \tag{16}$$

We first solve the eigenfunction $H_0(k_x,k_y,-i\partial_z)\Psi(x,y,z) = E_0(k_x,k_y)\Psi(x,y,z)$, which gives $E_0 = 0$ and

$$\Psi(x,y,z) = \mathcal{N}e^{ik_x x}e^{ik_y y}(e^{-\kappa_+ z} - e^{-\kappa_- z})\chi, \tag{17}$$

with $\mathcal{N}$ a normalization constant, $\chi = [\text{sgn}(k_y), -i]^T/\sqrt{2}$ and

$$\kappa_\pm = \frac{\lambda|k_y|}{2B} \pm \frac{i}{2B}\sqrt{4B\big(\tilde{m} - Bk_x^2 - Bk_y^2\big) - \lambda^2 k_y^2}. \tag{18}$$

The surface state exists only when $\min\{\text{Re}\kappa_+,\text{Re}\kappa_-\} > 0$, i.e., $k_x^2 + k_y^2 < \sqrt{\tilde{m}/B}$.

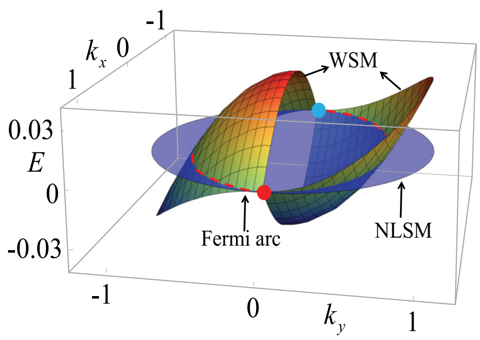

FIG. 3. The surface-state dispersions of the pristine crossing-nodal-line semimetal (flat surface) and the Floquet double-Weyl semimetal (tilted surfaces). The parameters are taken to be $m = B = \lambda = 1, \omega = 2, eA_0 = 0.2, \eta = 1, \phi = 0$, and $\theta = \pi/2$. The filled dots are the projections of double-Weyl points to the surface Brillouin zone. The red dashed lines are the two Fermi arcs connecting the two double-Weyl points (for zero chemical potential).

Now we add the perturbation ΔH, which modifies the dispersion as

$$\begin{aligned}\Delta E(k_x,k_y) &= \int_0^\infty dz\, \Psi^\dagger(x,y,z)\Delta H(k_x,k_y,-i\partial_z)\Psi(x,y,z)\\ &= \mathrm{sgn}(k_y)\gamma\eta\big[\big(\sin\phi\,\sin\theta k_x k_y - \cos\phi\,\sin\theta k_y^2\big)\\ &\quad + \kappa_+\kappa_-\cos\phi\,\sin\theta\big].\end{aligned} \tag{19}$$

Consequently, the surface states of the driven system become dispersive and the dispersion is given by $E(k_x,k_y) = \Delta E(k_x,k_y)$ in this perturbation theory. For the double-Weyl point case, i.e., $\theta = \pi/2$ and $\phi = 0$, the energy dispersion reads

$$E(k_x,k_y) = \mathrm{sgn}(k_y)\gamma\eta\big[\tilde{m}/B - k_x^2 - 2k_y^2\big]. \tag{20}$$

The surface-state dispersions of the pristine crossing-nodal-line semimetal and the Floquet double-Weyl semimetal are shown in Fig. 3. It is readily seen that the driving tears and tilts the flat drumhead surface band of the pristine NLSM, giving rise to two Fermi arcs. The number of Fermi arcs is equal to the monopole charge of the Weyl points.

Effect of spin-orbit coupling. Now we discuss the effect of spin-orbit coupling (SOC). As long as the pristine crossing structure is robust against SOC, such as that of the proposed material IrF_4 [58], where it is protected by nonsymmorphic symmetries, the introduction of SOC will only induce a change in the positions of the Flqouet Weyl points. On the other hand, if the pristine crossing structure is fragile to SOC, such as that of the candidate CaTe, where the nodal lines are predicated to evolve into Dirac points in the presence of SOC [123], we find the Floquet double-Weyl points become unstable and will be split into Floquet single-Weyl points (Supplemental Material).

Experimental estimations. Among other approaches, an optimal experimental method to verify this proposal is the pump-probe angle-resolved photoemission spectroscopy [102,104,105], which can directly measure the locations of double-Weyl points. Another approach is to measure the incident-angle-dependent Hall voltage, which is determined by the locations of the Floquet Weyl points [115,116]. Here we provide an estimation based on the material candidate Cu_3NPd [54,55]. Under the experimental condition of Ref. [102], γ is estimated to be of the order of 0.1λ, and a film sample with size $l_x \times l_y \times d = 100\ \mu\text{m} \times 100\ \mu\text{m} \times 500$ nm can generate an incident-angle-dependent Hall voltage of the order of 20 mV if a dc current of 100 mA is applied in y direction (Supplemental Material), well within the capacity of current experiments.

Conclusions. There have been extensive theoretical and experimental studies of Weyl points with monopole charge ± 1, however, multi-Weyl semimetals have not been well studied so far due to the lack of materials. Here, we show that multi-Weyl points can be realized in driven nodal-line semimetals with novel line connectivity (crossing nodal lines and nodal chains). In addition to suggesting a way to realize multi-Weyl semimetals, this work indicates that novel nodal lines are versatile platforms in the field of topological semimetals. Our proposal may also be generalized to cold-atom systems where periodic driving can be realized by shaking the optical lattice [134–136].

Note added. Recently, we became aware of a related preprint [137], in which type-I crossing is studied.

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