Nonequilibrium hybrid multi-Weyl semimetal phases

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Abstract

Multi-Weyl semimetals are variations of Weyl semimetals characterized by isolated band touching points, each carrying multiple topological charges. Given a plethora of exotic transport properties arising in such systems, it remains a longstanding interest to explore other variations of these semimetal phases. Of particular significance are hybrid multi-Weyl semimetal phases where many isolated band touching points, the number of which can be increased on-demand by tuning system parameters, carrying different topological charges coexist in the same setting. The experimental realization of such systems is expected to allow, in principle, clearer and more distinguishable signatures of isolated band touching points with various topological charges. In this work, we attempt to theoretically devise such systems by means of Floquet engineering. Specifically, we present three separate periodically driven systems displaying single-Weyl, double-single-Weyl, and triple-single-Weyl semimetal phases, each of which is capable of hosting a large number of isolated band touching points. We further report their intricate Fermi arc structures that result from the interplay between isolated band touching points of different charges. Moreover, we characterize these multi-Weyl nodes by use of a dynamical winding invariant.

1. Introduction

Weyl semimetals [1–6] emerged as a new paradigm in the study of topological matter, extending its classification beyond gapped systems such as topological insulators [7–10] and topological superconductors [11, 12]. Isolated band touching points with linear dispersion along all three quasimomenta, termed Weyl points, are hallmarks of such gapless topological matter. As a consequence of its topology, Weyl semimetals are known to display many intriguing phenomena [5, 13–19], which include, but not limited to, negative magnetoresistance [13], quantum anomalous Hall effect [20], and the chiral magnetic effect [21]. Weyl semimetals have also been experimentally observed in solid state materials [2, 6, 22–24], photonic [25, 26], optical [27–29], and acoustic [30, 31] systems.

Multi-Weyl semimetals [17, 19, 32–36], which have also been experimentally observed in [37–39], are variations of Weyl semimetals which exhibit isolated band touching points (multi-Weyl points) with linear dispersion along one direction and nonlinear dispersion along the other two directions (see figures 1(a)–(c)). Each multi-Weyl point carries multiple topological charges $Q > 1$ and chirality $\chi = \pm 1$, which can be understood as a result of $Q$ number of single-Weyl points of the same chirality $\chi$ coalescing at the same location in the three dimensional Brillouin zone [33, 34]. Under appropriate open boundary conditions, these multi-Weyl semimetal phases exhibit extended Fermi arc (figures 1(d)–(f)) spectrum [19, 33, 34, 38]. Moreover, a number of studies [40–45] have shown novel physical consequences of these multi-Weyl singularities for the simplest case of double-Weyl (charge $Q = 2$) semimetal phases. In view of these progresses, it is expected that other exotic variations of Weyl semimetals, such as those comprising of multiple isolated band touching points carrying different topological charges, give rise to previously undiscovered topological phenomena. Such hybrid multi-Weyl semimetals have been investigated in recent studies [46–49], where triple-, double-, and single-Weyl points [46] and double- and single-Weyl points [47–49] have been observed to coexist.
In this work, we systematically present variations of hybrid multi-Weyl semimetals capable of supporting arbitrarily many coexisting single-Weyl and multi-Weyl points of up to charge $Q = 3$. This is accomplished by the use of periodic driving, which places our systems at the heart of the timely area of Floquet topological matter [50–64]. Since the last decade, studies of Floquet topological matter have attracted attention due to the possibility of such systems to host exotic features with no static counterpart, which include topological edge states residing at half the driving frequency [58, 59, 62, 63], anomalous edge states not captured by any static topological invariants [53, 55, 57, 64–66], as well as the possibility of hosting a large number of edge states [56, 57, 60, 64, 67, 68]. While the hybrid multi-Weyl semimetal proposals of [47–49] also involve the use of periodic driving, the latter is only responsible for modifying the band structure of an otherwise trivial Hamiltonian into one that supports single- and multi-Weyl points. However, the number of single- and multi-Weyl points hosted by such systems remain fixed for a range of system parameters. By contrast, our periodic driving scheme is capable of exhibiting a large number of single- and multi-Weyl points that can be increased on-demand by tuning some system parameters. We expect such a feature to be desirable in experimental setting for achieving stronger signatures of single- and multi-Weyl points. In addition, as we will show below, the interplay among the various single- and multi-Weyl points leads to intricate Fermi arc structures, which may yield rich physical consequences.

The rest of this article is structured in the following way. In section 2, we introduce Floquet driving protocol and lattice models that exhibit hybrid multi-Weyl semimetal phases. We analytically locate the multi-Weyl nodes in our model systems and identify their charge and chirality by analysing the effective Hamiltonians. The charge and chirality of these multi-Weyl nodes serve as a benchmark for further calculations in identifying the topological invariant. More specifically, we discuss hybrid double-single and triple-single multi-Weyl semimetal phases in section 2.3 and section 2.4, respectively. We turn our focus towards the system’s surface state structures in section 3. We observe intricate Fermi arc structures arising from the interplay between single- and multi-Weyl nodes. Finally, we discuss the topological characterization of each individual multi-Weyl node in terms of the so-called dynamical winding number in section 4 before concluding in section 5.
2. Hybrid multi-Weyl semimetal phases

In this section, we present hybrid multi-Weyl semimetal phases where the double \((Q = 2)\) or triple \((Q = 3)\) multi-Weyl nodes coexist along with the single \((Q = 1)\) Weyl nodes. The proposed systems have the additional feature that the number of single- and multi-Weyl points can be made arbitrarily large by tuning some system parameters. To establish the intuition of our construction, we also present a more generic Floquet Weyl semimetal that only supports single-Weyl nodes, the number of which is controlled by some system parameters. For easier side-by-side comparison among them, we will describe the three systems simultaneously in the following.

2.1. Quench protocol, physical lattice models and symmetries

We consider non-interacting particles in three dimensions with two pseudo-spin degrees of freedom spanned by \(\sigma\); Pauli matrices. The (next) nearest neighbour hopping and on-site mass terms are modulated in such a way that each period of time consists of three intermediate quenches [56, 57]. During each step of the quench, the momentum space Hamiltonian \(H^{t}(k, t)\) only contains a single Pauli matrix, so that

\[
H^{t}(k, t) = \begin{cases} 
3\gamma^t_x(k)\sigma_x & T < t \leq T + \frac{T}{4} \\
3\gamma^t_y(k)\sigma_y & T + \frac{T}{4} < t \leq T + \frac{2T}{3} \\
3\gamma^t_z(k)\sigma_z & T + \frac{2T}{3} < t \leq 2T 
\end{cases},
\]

(1)

where \(T\) is the time-period of the drive and \(J \in [A, B, C]\) labels the system under consideration, i.e. \(A\) for a single-Weyl semimetal and \(B\) \((C)\) for a hybrid multi-Weyl semimetal with coexisting double- \((\text{ triple-})\) and single-Weyl points. We further take

\[
\gamma^t_x(k) = \begin{cases} 
t_x \sin(k_x) & \text{for } \gamma^t_x = A \\
t_x \sin(k_x) - \cos(k_y) & \text{for } \gamma^t_x = B \\
t_x \sin(k_y) [3\cos(k_x) - \cos(k_y) - 2] & \text{for } \gamma^t_x = C 
\end{cases},
\]

(2)

\[
\gamma^t_y(k) = \begin{cases} 
t_y \sin(k_y) & \text{for } \gamma^t_y = A \\
t_y \sin(k_y) \sin(k_y) & \text{for } \gamma^t_y = B \\
t_y \sin(k_y) [3\cos(k_x) - \cos(k_y) - 2] & \text{for } \gamma^t_y = C 
\end{cases},
\]

(3)

and \(\gamma^t_z = t_z + t_y \cos(k_x) + \cos(k_y) + t_y \cos(k_x) + t_y \cos(k_y) \cos(k_x) + \cos(k_x)\) for all \(J \in [A, B, C]\). Here \(t_i\)’s are the tunable system parameters that control the hopping strength and on-site mass term. By tuning various system parameters, each system exhibits distinct topological phases out of which we focus only on the Weyl semimetal phases in this study. The above models can potentially be realized experimentally in variations of the cubic optical lattices with tilted magnetic flux proposed in [69, 70]. Alternatively, they may also be simulated in one-dimensional waveguide arrays by introducing two additional periodic parameters \(k_x\) and \(k_y\) as synthetic dimensions [71, 72]. We would also like to highlight that such quench protocols are widely used [56, 57, 62, 64] due to their simple mathematical structure and that the obtained topological phases can survive upon smoothing out the idealized discontinuous quench protocols so as to be accessible in real experiments.

Time-periodic systems are treated in the framework of Floquet theory [73, 74]. Specifically, by diagonalizing the one-period time evolution operator (Floquet operator)

\[
U(k) \mid \Psi_n \rangle = e^{-i\frac{\Omega_n}{T}} \mid \Psi_n \rangle,
\]

(4)

where \(U(k) = e^{\hat{H}(k)dt} \hat{T}\) and \(\hat{T}\) being a time ordering operator, one obtains a set of Floquet eigenstates \(\mid \Psi_n \rangle\) and their corresponding quasienergies \(\Omega_n \in (-\pi / T, \pi / T]\) which are analogous to energy eigenstates and eigenvalues, respectively. The Floquet operator associated with the time-dependent system of equation (1) is given as

\[
U^{t}(k) = e^{-i\gamma^t_x\sigma_x} e^{-i\gamma^t_y\sigma_y} e^{-i\gamma^t_z\sigma_z},
\]

(5)

where we have fixed \(\hbar = T = 1\) for the rest of this article and \(J \in [A, B, C]\) labels the system under consideration, i.e. for \(s\) system with \(s = A, B, C\), the coefficients of Pauli matrices at the three time-steps are given as \(\gamma^t_x, \gamma^t_y\) and \(\gamma^t_z\).
By expanding out each exponential in equation (5), one obtains,

\[ U^\dagger(k) = d_0^\dagger \sigma_0 - i \left[ d_0^\dagger \sigma_x + d_y^\dagger \sigma_y + d_z^\dagger \sigma_z \right], \tag{6} \]

where \( d_i \)'s are functions of \( \gamma_i \)'s. The quasienergy is easily obtained as \( \Omega_{\pm} = \pm \cos^{-1} \left[ d_0^\dagger \right] \), where

\[ d_0^\dagger = \cos(\gamma_0^\dagger) \cos(\gamma_1^\dagger) \cos(\gamma_2^\dagger) + \sin(\gamma_0^\dagger) \sin(\gamma_1^\dagger) \sin(\gamma_2^\dagger). \tag{7} \]

All the systems introduced above possess the same three symmetries, i.e. charge-conjugation \( U_P U^\dagger(k, \ell) U_P^{-1} = U^\dagger(-k, T) \) and inversion \( U_F U^\dagger(k, \ell) U_F^{-1} = U^\dagger(-k, T) \). In particular, for systems labelled A and C, \( U_P = \sigma_x \) and \( U_F = \sigma_y \), whereas for B system, these symmetry operators are given as \( U_P = \sigma_y \) and \( U_F = \sigma_0 \), respectively [75]. The charge-conjugation symmetry ensures that the Weyl nodes in the system appear at either zero or \( \pi/T \) quasienergy while inversion symmetry implies that multi-Weyl nodes of opposite chirality are located at opposite momenta \( \pm k_0 \).

As we will elaborate further below, the three systems above support a number of isolated band touching points, around which the quasienergy dispersion is either linear (single-Weyl node), quadratic (double-Weyl node) or cubic (triple-Weyl node) in two specific spatial directions, while the third direction is always linear. Specifically, according to equation (7), we may identify the locations of these band touching points through the condition \( \gamma_0^\dagger = n_0 \pi \) or \( \gamma_i^\dagger = (n_i + 1/2) \pi \), where \( n_i \in \text{[integer]} \). Moreover, these band touching points emerge at quasienergy zero (\( \pi/T \)) if \( \gamma_i^\dagger \) further obeys the condition \( \sum_j \gamma_j^\dagger = 2m \pi \) \( (\sum_j \gamma_j^\dagger = (2m + 1) \pi) \) or \( \sum \gamma_j^\dagger = \pm 2m \pi \) \( (\sum \gamma_j^\dagger = -\pm 2m \pi) \) for \( m \) being an integer.

Before ending this section, it is worthwhile reviewing that a Hamiltonian describing an arbitrary multi-Weyl node of charge Q can be written as [19, 76],

\[ H_{\text{eff}}(k) = (k_x - ik_y)^0 \sigma_+ + (k_x + ik_y)^0 \sigma_- + \chi \kappa_\sigma_\gamma, \tag{8} \]

where \( \sigma_{\pm} = \frac{\sigma_x \pm i \sigma_y}{2} \), \( \chi \in \{1, -1\} \) is the chirality of multi-Weyl node and we have considered the unit Fermi velocity in all three dimensions.

2.2. Floquet Single-Weyl semimetal phases

To further elucidate our model construction, we first study the system described by the Hamiltonian \( H^\dagger(k, t) \) which only supports single-charge Weyl nodes. As a reminder to the reader, the piecewise Hamiltonian \( \gamma_i^\dagger \) at each time-step is given by \( \gamma_i^\dagger = t_s \sin(k_i \sigma_i) \), \( \gamma_i^\dagger = t_s \sin(k_i \sigma_i) \) and \( \gamma_i^\dagger = t_\sigma + t_\pi \cos(k_i \sigma_i) + t_\pi \cos(k_i \sigma_i) \). It is worth mentioning that the above model generalizes the 2D Floquet insulating model studied in [56, 57] which is capable of exhibiting an arbitrary number of co-propagating [56] and counter-propagating [57] edge states. We thus expect that, as further analytically confirmed below, the system presented here is also capable of hosting as many Weyl points as possible.

In order to analyse the system, we consider the quasi-momenta points where band crossings occur for \( \gamma_i^\dagger = n_i \pi \), \( \gamma_i^\dagger = n_i \pi \) and \( \gamma_i^\dagger = n_i \pi \), for \( n_i \in \text{[integer]} \). These conditions lead to the emergence of single-Weyl nodes at \( (k_x, k_y, k_\sigma) = \left( \sin^{-1} \left[ \frac{n_\pi}{\ell} \right], \sin^{-1} \left[ \frac{n_\pi}{\ell} \right] \pm \pi k_\sigma, 0 \right) \), \( (\pi - \sin^{-1} \left[ \frac{n_\pi}{\ell} \right], \sin^{-1} \left[ \frac{n_\pi}{\ell} \right], \pm k_\sigma, 0 \) and \( \pi - \sin^{-1} \left[ \frac{n_\pi}{\ell} \right], \pi - \sin^{-1} \left[ \frac{n_\pi}{\ell} \right] \pm \pi k_\sigma, 0 \) where \( k_\sigma = \cos^{-1} \left[ \frac{n_\pi - \beta \sigma}{\beta \sigma} \right] \) and \( \beta = \left[ 1 + \cos(k_i \sigma_i) + \cos(k_i \sigma_i) \right] \). In particular, note that as \( t_x \) or \( t_y \) increases by \( \pi \), there is a larger number of \( n_i \) or \( n_i \), for which \( \sin^{-1} \left[ \frac{n_\pi}{\ell} \right] \) or \( \sin^{-1} \left[ \frac{n_\pi}{\ell} \right] \) has a solution. Consequently, the proposed system is in principle capable of hosting as many Weyl points as possible, the number of which is tunable by parameters \( t_x \) or \( t_y \).

To further verify that the aforementioned band touching points correspond to single-charge Weyl points, one may explicitly expand the system’s Floquet operator near these points up to first order in \( \delta_i \), where \( (k_x, k_y, k_\sigma) = (k_0 + \delta_x, k_0 + \delta_y, k_0 + \delta_\sigma) \). The associated effective Hamiltonian \( H_{\text{eff}} = -\log \left[ U^\dagger(\delta) \right] \) is then obtained as

\[ H_{\text{eff}} = \left[ n_x + n_y + n_\pi \right] \pi \sigma_0 + \alpha_x \sqrt{t_x^2 - n_x^2 \pi^2 \delta_x \sigma_x} \]
\[ + \alpha_y \sqrt{t_y^2 - n_y^2 \pi^2 \delta_y \sigma_y} + \alpha_\pi \sqrt{t_\pi^2 - (n_\pi - \beta \sigma) \delta_\pi \sigma_\pi}, \tag{9} \]

where \( \alpha_i \in \{1, -1\} \). Band crossing at zero \( (\pi/T) \) quasienergy at these quasi-momenta occur at even (odd) values of \( \sum_i n_i \). The fact that \( H_{\text{eff}} \) is linear in all three dimensions confirms the expectation that \( (k_0, k_0, k_0) \) corresponds to a single-Weyl point, the chirality of which can be evaluated from \( H_{\text{eff}} \) through the usual
formula \( \chi = \text{sgn}[\prod \alpha_i] = \pm 1 \) [5]. We summarize the discussion of the present section with the numerical evaluation of the system’s quasienergy band structure (under periodic boundary conditions in all directions) at moderate values of \( t_x \) and \( t_y \) in figure 2. There, the emergence of various Weyl points at quasienergy zero and \( \pi/T \) quasienergy can be observed in the three dimensional Brillouin zone.

2.3. Floquet (pure) double and hybrid double-single-Weyl semimetal phases

In this section, we turn our attention to the system labelled as \( I = B \) in equation (1), which will be shown to support (pure) double- and hybrid (double-single-) Weyl semimetal phases. The Floquet operator \( U_B(k) \) of the time-periodic system is then obtained from equation (5) by taking \( \gamma_x^B = t_x \left( \cos(k_x) - \cos(k_y) \right) \), \( \gamma_y^B = t_y \sin(k_x) \sin(k_y) \) and \( \gamma_z^B = t_x + t_y \left( \cos(k_x) + \cos(k_y) \right) + t_0 \cos(k_z) + t_t \cos(k_z) \left( \cos(k_x) + \cos(k_y) \right) \). It is worth mentioning that the specific forms of \( \gamma_x^B \) and \( \gamma_y^B \) have been used as two Pauli components of static Hamiltonian exhibiting double-Weyl semimetal in previous literature [19, 76]. Here, we follow the same strategy above of separating \( \gamma_x^B \) and \( \gamma_y^B \) in two different time-steps to enable the generation of coexisting double- and single-Weyl points. In addition, we consider a different \( \sigma_z \) component \( \gamma_z^B \) as that of [19, 76] to enable the generation of many multi-Weyl points. As further detailed below, these in turn lead to a Floquet hybrid multi-Weyl semimetal capable of supporting a large number of coexisting single- and double-Weyl points.

We consider the band crossing condition \( \gamma_x^B = n_x \pi, \gamma_y^B = n_y \pi, \) and \( \gamma_z^B = n_z \pi \) which leads to the band touching points given as \( (k_x, k_y, k_z) = \left( \pm \cos^{-1} \left( \frac{n_x \pi - \beta \xi}{\alpha_x} \right), \pm \cos^{-1} \left( \frac{n_y \pi - \beta \xi}{\alpha_y} \right), \pm \cos^{-1} \left( \frac{n_z \pi - \beta \xi}{\alpha_z} \right) \right) \) where

\[
\alpha_x = \cos^{-1} \left( \frac{n_x \pi - \beta \xi}{\alpha_x} \right), \quad \xi = \pm \frac{n_x \pi}{t_x} + \frac{n_y \pi}{t_y}, \quad \text{and} \quad \xi = \pm \frac{n_z \pi}{t_z} + \frac{n_z \pi}{t_z},
\]

Here \( n_x \) takes (negative and non-negative) integer values while \( n_y \) takes only non-negative integer values such that the inequalities \( |\xi| \leq 1, |\xi| \leq 1 \) hold. Similarly, the solution under second condition, which is \( n_y = n_y = n_y = 0 \), can be obtained by taking \( n_y = n_y = 1/2 \) such that the inequalities \( |\xi| \leq 1, |\xi| \leq 1 \) hold for integer \( n_x, n_y \).

To quantitatively establish the above argument, we first consider small parameter values \( t_x = t_y = 1 \), so that \( n_x = n_y = 0 \) are the only allowed integer values for which \( \gamma_x^B = n_x \pi, \gamma_y^B = n_y \pi \) are solvable. This leads to several isolated band touching points at \( (k_x, k_y, k_z) = (0, 0, \pm k_x, 0) \) and \( (0, \pi, \pm k_x, 0) \), where

\[
k_x = \cos^{-1} \left( \frac{n_x \pi - \beta \xi}{\alpha_x} \right), \quad \beta = 1 + \cos(k_x) + \cos(k_y), \quad \text{and} \quad n_x \text{ take integer values such that}
\]
and chirality condition and linear (panels (e), (f)) dispersion in the show the quasienergy spectrum in the hybrid double-single-Weyl semimetal regime, where the coexistence of where \(\alpha\) is an integer such that the band touching points appear at zero (\(\pi/T\)) quasienergy for even (odd) values of \(n_z\). That is, the band touching points at above mentioned \((k_x, k_y, k_z)\) correspond to multi-Weyl points of charge \(Q = 2\) (as evidenced by the quadratic dispersion along the x and y directions) and chirality \(\chi = \text{sgn} [\prod \alpha_i] = \pm 1\). Moreover, note that the number of such double-Weyl points can be increased on-demand by tuning \(t_x\) and \(t_y\) parameter values, such that there are more integers \(n_z\) satisfying the condition \(-1 \leq \frac{n_z \pi - \beta t_0}{2\pi} \leq 1\). At these small values of \(t_x\) and \(t_y\), our system thus supports a (pure) double-Weyl semimetal phase exhibiting a potentially large number of double-Weyl nodes.

Next, by taking arbitrary values of \(t_x, t_y\), the previously identified double-Weyl points remain present at their respective locations, i.e. at \((k_x, k_y, k_z) = (0, 0, \pm k_{z,0})\) and \((\pi, \pi, \pm k_{z,0})\). However, additional isolated band touching points are formed at \((k_x, k_y, k_z) = (\pm \cos^{-1} \left[ \frac{\xi_{\gamma, \tau}}{k_x} \right], \pm \cos^{-1} \left[ \frac{\xi_{\gamma, \tau}}{k_y} \right], \pm k_{z,0})\), and \((\pm \cos^{-1} \left[ \frac{\xi_{\gamma, \tau}}{k_x} \right], \pm \cos^{-1} \left[ \frac{\xi_{\gamma, \tau}}{k_y} \right], \pm k_{z,0})\). By expanding the Floquet operator around these band touching points to the lowest order in \(\delta_{k}\), effective Hamiltonian is obtained as,

\[
H_{\text{eff}} = (n_x + n_y + n_z) \pi \sigma_0 + \left[ \cos(\xi_{\gamma, \pm}) \sin(\xi_{\gamma, \pm}) \delta_x + \cos(\xi_{\gamma, \pm}) \sin(\xi_{\gamma, \pm}) \delta_y \right] \sigma_y + \left[ -\sin(\xi_{\gamma, \pm}) \delta_x + \sin(\xi_{\gamma, \pm}) \delta_y \right] \sigma_x + \alpha_x \sqrt{\beta^2 t_0^2 - (n_x \pi - \beta t_0)^2} \delta_z \sigma_z,
\]

where \(\alpha_x \in \{+1, -1\}\). That is, the newly formed isolated band touching points represent single-Weyl nodes. With the coexistence of single- and double-Weyl points, our system thus represents a hybrid double-Weyl semimetal at these arbitrary larger values of \(t_x, t_y\). Moreover, while the number of double-Weyl points is tunable by the parameters \(t_x, t_y\) as elucidated above, the number of these additional single-Weyl points can also be increased on-demand via the parameter \(t_x, t_y\) through a similar mechanism.

By invoking the second condition above, i.e. \(n_x = (n_x + \frac{1}{2}) \pi, n_y = (n_y + \frac{1}{2}) \pi\) and \(n_z = (n_z + \frac{1}{2}) \pi\), additional band touching points are found at \((k_x, k_y, k_z) = (\pm \cos^{-1} \left[ \frac{\xi_{\gamma, \pm}}{k_x} \right], \pm \cos^{-1} \left[ \frac{\xi_{\gamma, \pm}}{k_y} \right], \pm k_{z,0})\), and \((\pm \cos^{-1} \left[ \frac{\xi_{\gamma, \pm}}{k_x} \right], \pm \cos^{-1} \left[ \frac{\xi_{\gamma, \pm}}{k_y} \right], \pm k_{z,0})\). Expanding the Floquet operator around these band touching points result in effective Hamiltonian similar to equation (11) by taking \(\xi_{\gamma, \pm} = \frac{\xi_{\gamma, \pm}}{k_{x, \pm}}\) and \(\sqrt{\beta^2 t_0^2 - (n_x \pi - \beta t_0)^2}\) instead of \(\xi_{\gamma, \tau} = \frac{\xi_{\gamma, \tau}}{k_{x, \pm}}\) and \(\sqrt{\beta^2 t_0^2 - (n_x \pi - \beta t_0)^2}\), respectively.

Combining all the analyses above, it follows that the system \(H^\theta(\mathbf{k}, t)\) supports a (pure) double-Weyl semimetal phase at small \(t_x, t_y < \pi/2\), while it becomes a hybrid double-single-Weyl semimetal at large \(t_x > \pi/2\) or \(t_y > \pi/2\). The number of double- (single-) Weyl points can be increased on-demand through the parameters \(t_x, t_y\). To complement these analytical treatments, we numerically evaluate the system’s quasienergy spectrum under periodic boundary conditions in all spatial directions and present our results in figure 3. Specifically, the quasienergy spectrum in the (pure) double-Weyl semimetal regime, which only supports double-Weyl points, can be observed in figures 3(a) and (b). In figures 3(c)–(f), we further show the quasienergy spectrum in the hybrid double-single-Weyl semimetal regime, where the coexistence of double- and single-Weyl points is clearly observed as band touching points exhibit quadratic (panels (c), (d)) and linear (panels (e), (f)) dispersion in the \(k_x - k_y\) direction, respectively.

2.4. Floquet hybrid triple-single-Weyl semimetal phases

In this section, we analyse the system labelled as \(J = C\) in equation (1), characterized by the Hamiltonian components \(\gamma_x^C = t_x \sin(k_x) [3 \cos(k_x) - \cos(k_x) - 2]\), \(\gamma_y^C = t_y \sin(k_y) [3 \cos(k_y) - \cos(k_y) - 2]\) and \(\gamma_z^C = t_z \sin(k_z) [3 \cos(k_z) - \cos(k_z) - 2]\). We further take \(t_x = t_y = 1\) for simplicity. By employing the same strategy as before, we identify the locations of isolated band touching points by first invoking the condition \(\gamma^C = n_x \pi, \gamma^C = n_y \pi, \gamma^C = n_z \pi\) and \(\gamma^C = n_x, n_y, n_z\), where \(n_x, n_y, n_z\) are integers. By taking \(n_x = n_y = 0\), these isolated band touching points are located at \((k_x, k_y, k_z) = (0, 0, \pm k_{z,0}), (0, \pi, \pm k_{z,0}), (\pi, 0, \pm k_{z,0}), (\pi, \pi, \pm k_{z,0})\), where \(k_{z,0} = \cos^{-1} \left[ \frac{n_z \pi - \beta t_0}{2\pi} \right]\) by expanding the Floquet
operator around the point \((0, 0, \pm k_z, 0)\) up to the lowest order in \(\delta_i\)’s, the associated effective Hamiltonian \(H_{\text{eff}} = -i\log[U^\tau(k)]\) is found to be of triple-Weyl Hamiltonian form, i.e.

\[
H_{\text{eff}} = n_z \pi \sigma_0 + \frac{k}{2} \text{Re}[(\delta_x - i \delta_y) \sigma_x] - \frac{f_y}{2} \text{Im}[(\delta_x - i \delta_y) \sigma_y] + \sqrt{\beta^2 f_y^2 - (n_z \pi - \beta t_b)^2} \delta_z \sigma_z,
\]

where \(\beta = [1 + \cos(k_x) + \cos(k_y)]\). That is, the point \((0, 0, \pm k_z, 0)\) represents a triple-Weyl point. By expanding the Floquet operator around the remaining three points, i.e. \((k_0, k_y, k_z) = (0, \pi, \pm k_z, 0),\)

\((\pi, 0, \pm k_z, 0)\) and \((\pi, \pi, \pm k_z, 0)\), we obtain effective Hamiltonian of the form

Figure 3. Quasienergy spectrum of system \(U^\tau\) under periodic boundary conditions in all spatial directions has been shown for parameter values (a), (b) \(t_x = t_y = 1, t_z = 4\pi/3, \ t_b = 3.5, \) for (a) \(k_z = \pm \pi, \ t_a = 0, \ t_b = 0.8\pi, \)

\(t_x = 1, \ t_y = \pi, \ t_z = 2.5\) for (c) \(k_z = 0\) (d) \(k_z = \pi/2\) and (e), (f) \(t_x = 1, \ t_y = \frac{8\pi}{16}, \ t_z = \pi, \ t_b = 2.5\) for (c) \(k_z = 0.339\pi\) (f) \(k_z = 0.284\pi\). Panels (a), (b) show the pure double-Weyl semimetal phase while (c)–(f) show the hybrid (double-single-) Weyl semimetal phases.
Quasienergy spectrum of system $U_0(k)$ under periodic boundary conditions has been shown for fixed parameter values $t_x = t_y = 1$, $t_z = 2.5$ for (a) $k_x = 0$ (b) $k_x = 0$ (c) $k_z = 0$ and (d) $k_z = 0.795\pi$. Multi-Weyl node of charge $Q = 3$ with cubic quasienergy dispersion can be observed (b) for $(k_x, k_y) = (0, 0)$ at zero and $n/1$ quasienergy. Moreover, (a)–(d) show that the system support Weyl nodes of charge $Q = 3$ and $Q = 1$ at various momenta points in the three dimensional Brillouin zone.

\[
H_{\text{eff}} = n_x \pi \sigma_0 + \beta_x \delta_0 \sigma_x + \beta_y \delta_y \sigma_y + \sqrt{\beta^2 t_y^2 - (n_z \pi - \beta t_x)^2} \delta_z \sigma_z ,
\]

for $(\beta_x, \beta_y) = (-6, -4), (-4, -6)$ and $(4, 4)$, respectively. That is, these three points correspond to single-Weyl points.

By taking $n_x = \pm 1$ and $n_y = 0$ in the condition above, additional isolated band touching points are found at $(k_{x_0}, k_{y_0}, k_{z_0}) = (\pm 2 \tan^{-1}[8/9\pi], \pi, \pm k_{z,0})$, $(\pm 2 \tan^{-1}[66/9\pi], \pi, \pm k_{z,0})$ and $(\pm 2 \tan^{-1}[42/9\pi], \pm 2 \tan^{-1}[66/9\pi], \pm k_{z,0})$. In a similar fashion, taking $n_x = 0$ and $n_y = \pm 1$ leads to isolated band touching points at $(k_{x_0}, k_{y_0}, k_{z_0}) = (\pi, \pm 2 \tan^{-1}[8/9\pi], \pm k_{z,0})$, $(\pi, \pm 2 \tan^{-1}[66/9\pi], \pm k_{z,0})$ and $(\pm 2 \tan^{-1}[42/9\pi], \pm 2 \tan^{-1}[16/9\pi], \pm k_{z,0})$. Moreover, the condition $\gamma_{yC}^C = (n_x + \frac{1}{2})\pi$, $\gamma_{yF}^C = (n_y + \frac{1}{2})\pi$ and $\gamma_{zF}^C = (n_z + \frac{1}{2})\pi$ further leads to isolated band touching points at $(k_{x_0}, k_{y_0}, k_{z_0}) = (\pm 2 \tan^{-1}[128/9\pi], \pm 2 \tan^{-1}[128/9\pi], \pm k_{z,0}^F)$ and $\beta = [1 + \cos(k_{y_0}) + \cos(k_{y_0})]$. By expanding the Floquet operator around each of these additional isolated band touching points and writing down the associated effective Hamiltonian, we find that they represent single-Weyl points.

Unlike $J = B$ system considered in the previous section, we thus find that $J = C$ system already represents a hybrid multi-Weyl semimetal with coexisting triple- and single-Weyl points even in the regime of small $t_x$ and $t_y$. Note however that, similar to $J = B$ system, the number of these Weyl points can be increased on-demand by tuning system parameters $t_x, t_y, t_a$ and $t_b$, which leads to a larger number of allowable integers $n_x, n_y, n_z$ for which the above band touching conditions can be satisfied. Finally, in figure 4, we plot the system’s quasienergy spectrum under periodic boundary conditions at several quasienergy slices to explicitly demonstrate the emergence of multiple single- and triple-Weyl points elucidated above.
3. Surface state structures

Having identified the location and nature of various Weyl points in all the systems presented above, we will now investigate the implication of their topology through extensive numerical band structure studies of the three systems under open boundary conditions along one of the three spatial directions. It can be observed that the above systems are symmetric in $k_x$ and $k_y$ (at $t_x = t_y$); opening either $x$ or $y$ direction will result in similar surface state (Fermi arc) structures. As such, we only consider open boundary conditions in $x$-direction and periodic boundary conditions in the $y$ and $z$ direction for all systems in the remainder of this section.

We start by plotting the surface state structures of the single-Weyl semimetal system ($J = A$) in figure 5, where each panel represents either zero or $\pi/T$ quasienergy cut only. There, red dots indicate the projection of single-Weyl nodes in the $k_y - k_z$ plane. As expected, dispersionless Fermi arcs [2–5, 22, 23, 62] connecting each pair of these single Weyl nodes along a straight line are clearly observed. These Fermi arcs can be non-, doubly or triply degenerate depending on the number of single-Weyl nodes near their end points (labelled by (1)–(3) in figure 5). Here, each Fermi arc contains two-fold degenerate surface states, so that non-, doubly or triply degenerate Fermi arcs correspond to two-fold, four-fold, and six-fold degenerate surface states.

Next, we turn our attention to the second system ($J = B$) corresponding to either (pure) double-Weyl semimetal or hybrid double-single-Weyl semimetal depending on the system parameters. In figure 6, we plot the typical surface state structures at zero and $\pi/T$ quasienergy cuts for three different representative parameter values. Unlike single-Weyl nodes, a pair of double-Weyl nodes is connected by a pair of curved Fermi arcs, which together form a circular shaped structure [32–34, 38, 42] as shown in figure 6(a). More interestingly, in the hybrid multi-Weyl semimetal setting, we find that the Fermi arcs connecting a pair of single-Weyl points may no longer form the same straight line. In some cases, these Fermi arcs may form a circular shape that becomes indistinguishable from those connecting a pair of double-Weyl points. Such circular shaped Fermi arcs occur in the presence of multiple single-Weyl points separated in the $x$ direction, which are thus projected onto the same point in the $k_y - k_z$ plane. Due to the interplay between the various single- and multi-Weyl points, the Fermi arcs associated with different pairs of these single-Weyl points no longer form the same straight line and instead form different curves that together make up such a circle-like shape. As shown in figures 6(e) and (f), the Fermi arcs associated with the double-Weyl points may also take a compressed elliptical or butterfly-like structure. To our knowledge, such intricate Fermi arc structures have
Figure 6. A quasienergy (a), (c), (e) zero and (b), (d), (f) $\pi/T$ slice of system $U^B$ under open (periodic) boundary conditions along $x$ ($y$ and $z$)-direction has been shown for parameter values (a), (b) $t_x = t_y = 1$, $t_a = 4\pi/3$, $t_b = 3.5$, (c), (d) $t_x = 0.8\pi$, $t_y = 1$, $t_a = \pi$, $t_b = 2.5$ and (e), (f) $t_x = 1$, $t_y = \frac{8\pi}{16} - \pi$, $t_a = \pi$, $t_b = 2.5$. Projection of charge $Q = 2$ (green) and $Q = 1$ (red) Weyl nodes onto the $k_y - k_z$ quasimomenta plane has been shown, where the associated Fermi arcs are presented in blue.

not been reported and require the presence of many single- and multi-Weyl points. Indeed, while the experiment of [46] also studies a system with coexisting single- and multi-Weyl points, the low number of Weyl points does not give rise to anomalous Fermi arc structures discussed above.

Finally, we present the surface state structures of the third system ($J = C$) in figure 7 for various parameter values. The projection of triple- (single-) Weyl nodes in $k_y - k_z$ momenta plane has been shown in magenta (red) dots at zero or $\pi/T$ quasienergy slice in figures 7(a), (c) and (e) or figures 7(b), (d) and (f), respectively. Similarly to the Floquet hybrid double-single-Weyl semimetal phase discussed above, due to the coexistence of triple- and single-Weyl points, intricate Fermi arc structures connecting different pairs of multi-Weyl points are observed. An interesting observation can be made in figures 7(d) and (f), where outermost triple-Weyl nodes have disparate surface states structure such that circular and linear surface states flow in the opposite $k_z$-direction (the magenta arrows in figures 7(d) and (f). That is, linear (circular) part of the
surface states of these triple-Weyl nodes flow through $k_z = 0 \ (\pi)$ to connect their counterparts with opposite chirality. Significant difference between conventional and disparate surface states of triple-Weyl nodes can be observed in figures 7(d) and (f) where black and magenta arrows follow the flow of these surface states. Moreover, the surface states of triple- (double-) Weyl nodes intersect the surface states associated with single-Weyl nodes such that the degeneracy of the surface states add up at these intersecting points. A few of these intersecting points ($\Lambda$) are shown in figure 6(c) and figures 7(d) and (f). These observations of intricate surface state structures add knowledge to the hybrid multi-Weyl semimetal phases and may lead to unforeseen exotic transport properties. Further exploration of the latter forms an interesting aspect for future work.
4. Topological characterization of hybrid-multi Weyl phases

Static multi-Weyl semimetal phases have been characterized in terms of a Chern number over a closed surface surrounding one of the multi-Weyl nodes [33]. Such a Chern number captures the charge of the enclosed Weyl point, thus distinguishing single-Weyl points from their larger-charged counterparts. While such a Chern number characterization can in principle be adapted to the time-periodic setting, the presence of arbitrarily many Weyl points [63, 64] in some systems may hinder their practical feasibility, i.e. creating a sufficiently small surface enclosing a single Weyl point is challenging. In Chern multi-Weyl semimetal phases [32], i.e. systems which can be written as a stack of Chern insulators, slice Chern number procedure can also be employed. This amounts to scanning the Chern number over two-dimensional slices of the three-dimensional Brillouin zone. In such a procedure, the jump in the Chern number values is identified with the presence of multi-Weyl points. However, the drawback with such a procedure is that it may fail altogether when multiple Weyl points occur at a two-dimensional slice of the three-dimensional Brillouin zone, which is often the case in the systems considered in this paper.

In our previous work [64], we employ dynamical winding characterization to distinguish various Weyl points at zero and \( \pi/T \) quasienergies in a Floquet single-Weyl semimetal system. In the following, we will show that such a dynamical winding procedure can also distinguish Weyl points of different charges.

We begin our analysis of dynamical winding number by identifying that a generic Floquet operator around a multi-Weyl node of charge \( Q \) can be written as, using equation (8),

\[
U^Q = \cos(m \pi) \sigma_0 - i(k_x - i k_y) \sigma_+ - i(k_x + i k_y) \sigma_- - i \chi k_x \sigma_z ,
\]

where \( \sigma_{\pm} = \frac{\sigma_+ \pm i \sigma_-}{2} \), \( \chi \in \{ +1, -1 \} \) is the chirality of multi-Weyl node and \( m \) takes even (odd) values for multi-Weyl nodes at zero \( \pi/T \) quasienergy. We then consider a Cartesian to spherical co-ordinate transformation such that \( k_x = \text{rsin} \theta \cos \phi \), \( k_y = \text{rsin} \theta \sin \phi \) and \( k_z = \cos \theta \), where \( r \) is the radius of the sphere, \( \theta \in [0, \pi] \) and \( \phi \in [0, 2\pi] \) are the polar and azimuthal angles respectively. The dynamical winding number over the closed 2D surface defined by the sphere of radius \( r \) is then given as [55, 64],

\[
W^r = \frac{1}{8\pi^2} \int_0^T \int d\theta \, d\phi \left[ \hat{U}_r \right] \times \text{Tr} \left[ \hat{U}_r^{-1} \hat{U}_r^{Q} \hat{U}_r^{-1} \hat{U}_r^{Q} \hat{U}_r^{-1} \hat{U}_r^{Q} \right] ,
\]

where \( \varepsilon \) is the branch cut of the logarithmic function and the modified Floquet operator \( \hat{U}_r^{Q} \) is given as,

\[
\hat{U}_r^{Q} = \begin{cases} 
U_r^{Q}(\Theta, 2t) & \text{if } 0 \leq t < T/2 \\
(\exp\left(-\frac{i}{\Omega_1} t\right))^{2m} & \text{if } T/2 \leq t < T 
\end{cases},
\]

where \( \Omega_1^{Q} = -i \log \left[ U^Q \right] \) is the effective Hamiltonian of the system, \( \Theta = (\theta, \phi) \) and \( T \) is the driving period. The modified Floquet operator during the second half of the time-period is given as,

\[
\hat{U}_r = \left( \frac{1}{2} \left[ e^{-\Omega_{1}^{Q} t} (1 + M) + e^{-\Omega_{2}^{Q} t} (1 - M) \right] N (e^{-\Omega_{1}^{Q} t} - e^{-\Omega_{2}^{Q} t}) \right) \frac{1}{2} \left[ e^{-\Omega_{1}^{Q} t} (1 - M) + e^{-\Omega_{2}^{Q} t} (1 + M) \right]
\]

for \( M = \frac{\chi \cos(\theta) \sin(m \theta)}{\sqrt{\cos^2(\theta) + \sin^2(m \theta)}} \) and \( N = \frac{\chi \cos(\theta) \sin(m \theta)}{2\sqrt{\cos^2(\theta) + \sin^2(m \theta)}} \). The contribution towards the dynamical winding number of the time interval \( 0 \leq t < T/2 \) is zero up to \( Q^{th} \) order approximation in \( r \) such that terms with \( r^{Q+1} \) and higher power are neglected. This can be explicitly checked by evaluating equation (15). The contribution of the second half is then obtained by directly integrating equation (15) in the interval \( T/2 \leq t < T \), which results in,

\[
W^r = \chi Q \cos(m \pi) \Omega_2^r - \Omega_1^r - \sin(\Omega_2^r - \Omega_1^r) \frac{2\pi}{\Omega_1^r} .
\]

Therefore, \( W^r = \chi Q \) for \( m = 2m' \) since \( \Omega_1^r = -2\pi + \tan^{-1}(f(r)) \) and \( \Omega_2^r = -\pi - \tan^{-1}(f(r)) \). On the other hand, we obtain \( W^r = \chi Q \) for \( m = (2m' + 1) \) since quasienergy \( \Omega_1^r = \pi - \tan^{-1}(f(r)) \) and \( \Omega_2^r = -\pi + \tan^{-1}(f(r)) \). The function \( f(r) \) is a \( Q \) dependent function of \( r \) such that \( \sin^{-1}(f(r)) \to 0 \) and \( \cos^{-1}(f(r)) \to 1 \) for small \( r \). In summary, the dynamical winding number effectively captures a multi-Weyl node of any charge \( Q \) and chirality \( \chi \) at zero and \( \pi/T \) quasienergy.
Table 1. System parameters are taken as $t_x = t_y = 1$, $t_z = \pi$, $t_\nu = 2.5$ for $\Delta_1 - \Delta_9$ and $t_x = t_y = 0.8\pi$, $t_z = \pi$, $t_\nu = 2.5$ for $\Delta_1 - \Delta_{10}$ where $\Delta_i$ represent different cases. We consider a closed 2D spherical surface enclosing the multi-Weyl node under consideration and determine the associated charge and chirality in the form of dynamical winding number ($W^q$, $W^\pi$) evaluated from Floquet operator.

Charge and chirality of the Weyl nodes $(\chi Q)^*\epsilon$ at $\epsilon$ quasieenergy are directly derived from analytical solutions of the effective Hamiltonian associated with each multi-Weyl node enclosed. We have defined $\mu_\chi = \cos^{-1}(\Delta_n/\muQ)\pi$ where $\mu_n$ takes even or odd non-negative integer values and $\beta = 1 + \cos(k_x) + \cos(k_y)$.

| $\Delta_i$ | $J$ | $r$ | $(k_{x_0}, k_{y_0})$ | $(\chi Q)^*$ | $(W^q, W^\pi)$ |
|-----------|-----|-----|----------------------|-------------|--------------|
| $\Delta_1$ | $A$ | 0.35 | $(0, 0, \pm \mu_{even})$ | $(-1)^0$ | $(\mp 1, 0)$ |
| $\Delta_2$ | $A$ | 0.35 | $(0, 0, \pm \mu_{odd})$ | $(-1)^\pi$ | $(0, \mp 1)$ |
| $\Delta_3$ | $B$ | 0.35 | $(0, 0, \pm \mu_{even})$ | $(+2)^0$ | $(\pm 2, 0)$ |
| $\Delta_4$ | $B$ | 0.35 | $(0, 0, \pm \mu_{odd})$ | $(+2)^\pi$ | $(0, \pm 2)$ |
| $\Delta_5$ | $C$ | 0.35 | $(0, 0, \pm \mu_{even})$ | $(+3)^0$ | $(\pm 3, 0)$ |
| $\Delta_6$ | $C$ | 0.35 | $(0, 0, \pm \mu_{odd})$ | $(+3)^\pi$ | $(0, \pm 3)$ |
| $\Delta_7$ | $C$ | 0.25 | $(0.62\pi, 0.32\pi, \pm \mu_{even})$ | $(+1)^0$ | $(\pm 1, 0)$ |
| $\Delta_8$ | $C$ | 0.25 | $(0.62\pi, 0.32\pi, \pm \mu_{odd})$ | $(+1)^\pi$ | $(0, \pm 1)$ |
| $\Delta_9$ | $B$ | 0.10 | $(0.58\pi, 0, \pm \mu_{odd})$ | $(+1)^0$ | $(\pm 1, 0)$ |
| $\Delta_{10}$ | $B$ | 0.10 | $(0.58\pi, 0, \pm \mu_{even})$ | $(+1)^\pi$ | $(0, \pm 1)$ |

We now turn our attention towards numerical results of dynamical winding number in the models presented in section 2 and summarize our results in table 1. In order to numerically calculate the dynamical winding invariant, we consider 2D spherical closed surface parameterized by $\theta$ and $\phi$ such that $k_x = k_{x_0} + r \sin(\phi) \cos(\theta)$, $k_y = k_{y_0} + r \sin(\phi) \sin(\theta)$ and $k_z = k_{z_0} + r \cos(\theta)$ where $(k_{x_0}, k_{y_0}, k_{z_0})$ is a Weyl node of charge $Q$ and chirality $\chi$. Table 1 represents numerical results of dynamical winding number ($W^q$, $W^\pi$) obtained from Floquet operator while charge and chirality $(\chi Q)^*$ of multi-Weyl nodes at quasienergy $\epsilon$ evaluated from effective Hamiltonian description. $\Delta_1$ ($\Delta_2$) in table 1 represents the single-Weyl nodes at zero ($\pi/T$) quasienergy associated with system $A$. Second, $\Delta_3 - \Delta_4$ and $\Delta_9 - \Delta_{10}$ respectively represent double- and single-Weyl nodes associated with system $B$. Finally, $\Delta_5 - \Delta_6$ and $\Delta_7 - \Delta_8$ respectively describe triple- and single-Weyl nodes associated with system $C$. It follows that these numerical results agree with our analytical prediction that dynamical winding number effectively captures the charge and chirality of triple-, double-, and single-Weyl nodes at zero and $\pi/T$ quasienergy.

5. Concluding remarks

In this article, we have proposed several Floquet hybrid multi-Weyl semimetal phases where arbitrarily many double (triple) Weyl nodes and single Weyl nodes may coexist. The locations of these Weyl points were analytically identified by studying the systems’ Floquet operator, and their charges were then determined by expanding such a Floquet operator around these locations. To verify these Weyl nodes topology, we also studied the surface state structures of the systems. Due to the interplay between single- and (double-) triple-Weyl points, intricate Fermi arc structures connecting pairs of these Weyl points are obtained. Finally, we discussed the topological characterization of the three systems in terms of dynamical winding number.

In the future, it will be interesting to explore the physical consequences of the various Fermi arc structures discovered here on the systems’ transport properties. Moreover, creating Floquet hybrid multi-Weyl semimetal phases with a large number of coexisting triple, double and single Weyl nodes may also present an opportunity for accessing potentially richer and previously undiscovered Fermi arc structures.

Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

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