On the topological character of three-dimensional Nexus triple point degeneracies

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Recently a generic class of three-dimensional band structures was identified (Chang et al, Scientific reports \textbf{7}, 1 (2017)) that host two-fold line degeneracies that meet at three-fold or triple point degeneracies, which resist the usual topological characterization of isolated point degeneracies as in Dirac/Weyl semimetals. For these so-called “Nexus” fermions which lie beyond Dirac/Weyl fermions, we lay out several concepts to characterize the wavefunction geometry and spell out its topology. Our approach is based on an understanding of the analyticity properties of the Nexus wavefunctions building on a two-dimensional analogue studied in Phys. Rev. B \textbf{100}, 125152 (2019). We use this to write down a homological classification of various Nexus triple point degeneracies in three dimensions.

I. INTRODUCTION

Band theory of electronic structure occupies a venerable place in quantum condensed matter. Historically, the basic ideas were established quite soon after the development of quantum mechanics. Yet, it is still an active area of research even in the current day with many surprises. Among the surprises, topological band insulators and superconductors have captured our imagination in a big way\textsuperscript{12}. They had their antecedent in the integer quantum Hall effect\textsuperscript{8,10}. The electronic structure of these quantum states of matter have interesting and robust phenomenology, e.g. the edge states of topological bands\textsuperscript{4,5}. Another surprise has been the wealth of physics present in two and three dimensional (2d and 3d) semimetals\textsuperscript{5,10}. The low energy excitations in semimetals also often possess a topological character. This can lead to a certain robustness against back-scattering\textsuperscript{11}. Already the low density of semimetallic carriers at the Fermi energy makes the effect of interactions less relevant. The combination of these two effects holds great promise for potential applications of semimetals\textsuperscript{8}.

From a theoretical point of view, what gives the semimetallic carriers their topological character is the global structure of the wavefunction geometry of the electronic bands. Dirac and Weyl semimetals are the well-known examples in 2d and 3d. These semimetals have two-fold degeneracies at points in the Brillouin zone often protected by certain symmetries\textsuperscript{10}. The semimetallic character obtains when the Fermi energy is near these degeneracies. Such two-fold point degeneracies are generic only in 3d, while they are exceptional in 2d thus requiring symmetry protection\textsuperscript{10}. Recently, generalization of Dirac and Weyl fermions have also been found by symmetry-protecting higher-fold point degeneracies\textsuperscript{11}.

While there has been tremendous activity on semimetals with point degeneracies, it has also been realized that band structures with two-fold line degeneracies are another possibility in the universe of possible band structures. Line degeneracies are exceptional in 3d, and symmetry protection is required to obtain them. Several symmetry protected possibilities have been identified recently\textsuperscript{12,13}. Among these there is a class of band structures where two-fold line degeneracies meet at three-fold or triple point degeneracies. They have been dubbed as Nexus fermions\textsuperscript{13,14}. There have been material proposals\textsuperscript{15,17,22} and experimental observations\textsuperscript{22,23} on this class of fermions. The spectral structure of this class of fermions is intriguing, and their band topology has been analysed previously in terms of the line degeneracies and \(Z_2\) topological number\textsuperscript{22}. The goal of this paper is to shed more light on the band topology of Nexus fermions in a different manner which particularly emphasizes classifying the topology of the Nexus triple points as defects in the space of band wavefunctions.

The topological character of point degeneracies can be understood by studying the band topology in one lower dimension\textsuperscript{22}. One generally considers a surface in the momentum space that encloses the 3d point degeneracy in question. Since the surface can be chosen to be gapped everywhere, one then computes the Chern number on this surface which serves as a topological charge for the point degeneracy. This discrete topological charge can not be changed by small deformations to the Hamiltonian. This approach will fail for characterizing the Nexus triple point degeneracy, because any surface enclosing the triple point degeneracy will have gapless points where the line degeneracies intersect with the chosen surface. Thus the general principle of calculating a topological charge on an enclosing surface will not work.

This is why Ref.\textsuperscript{15} called the Nexus system they introduced as a “beyond-Weyl” system.

If we restrict ourselves to use only gapped lower dimensional spaces, one can at best characterize the topology of the line degeneracies by considering gapped loops around them\textsuperscript{14,16,22}. The question then is how to proceed in order to characterize the wavefunction geometry of a Nexus system including the basic issue of whether Nexus triple points have a topological character or not. This is a relevant question not just as a conceptual issue, but also because of the following physical point: in Weyl systems, the surface Fermi arcs have a protection in the sense that they have to end at the projection of the bulk Weyl points on to the surface\textsuperscript{22}. This protection is linked to
the fact that the Weyl points in the bulk possess a topological character. Ref.\textsuperscript{13} raised the analogous question on whether the surface Fermi arcs numerically observed in their chosen Nexus systems have a protection in the sense of Weyl Fermi arcs. This would be the case if the Nexus triple points have topological character. See the discussion on the Nexus Fermi arcs in Ref.\textsuperscript{13} for more on this point. Our paper gives a constructive method to capture the topological character of different Nexus triple points. This method is the main result of this paper. Thus, we give an affirmative answer to the question raised in Ref.\textsuperscript{13}, i.e. there will be surface Fermi arcs in Nexus systems that will have to end at the projection of the bulk triple points on to surface.

Our method relies crucially on the analytic properties of the band wavefunctions near the line degeneracies. This builds on the results of Ref.\textsuperscript{26} where a toy 2d band structure was considered which had a certain likeness to the Nexus band structures. In particular, specific 2d cuts of some Nexus band structure resembles the toy band structure considered in Ref.\textsuperscript{26}. The wavefunctions of this toy model were explicitly written down which made the band topology explicit as well. The 2d topology could be captured by a generalization of winding number\textsuperscript{25,27}.

This was based on an understanding of the analyticity properties near the line degeneracies. This taught us the bigger lesson that near line degeneracies, analytic continuation or movement in the space of wavefunctions is key to exposing the band topology.

Motivated by the above, we will study in detail the analyticity properties of several 3d Nexus band structures. We will use Dirac and Weyl systems as scaffolding for the analyticity discussions of Nexus band structures. In the process, we will come to an important notion of the generalized parameter domain when dealing with degeneracies. This will be necessitated by the presence of degenerate points on the surface enclosing the Nexus triple point degeneracy. For point degeneracies like Weyl points, this notion is not necessitated because we can easily find a gapped surface to surround the Weyl point.

Equipped with the generalized parameter domain, we can finally state data on the band topology of a Nexus band structure. This scheme will consist of specifying and counting the distinct analytic loops that can be drawn on the generalized domain around a triple point. Thus we will have the desired scheme to distinguish different triple point degeneracies based on their distinct band topology data. This idea is very similar to the homology classes of 1-cycles used to distinguish the topology of different geometric objects. The familiar example is that of a sphere vs. a torus. The sphere admits no loops that can’t be contracted to a point, whereas a torus admits two distinct classes of loops that can’t be contracted to a point. Our scheme will do a similar classification of the triple points, with the structure of homology classes being dictated by the structure of line degeneracies. In this way, we will be able to classify several Nexus band structures written down in the literature\textsuperscript{13} as well as some obtained as 3d extensions of the toy band structure in Ref.\textsuperscript{29}. This classification is the culminating result of this paper. Furthermore, this scheme can also potentially reveal the inter-relationships between the different kinds of triple points.

We give a brief outline of the paper: Sec. \textsuperscript{II} sets the stage by recapitulating some 2d band structures from the point of view of analyticity. We will be paying close attention to what happens near degeneracies, since that is the main roadblock in understanding the band topology of Nexus band structures. Doing this will introduce the notion of the generalized domain. We then go on 3d in Sec. \textsuperscript{III} where we start by discussing the familiar Weyl system to give a clear contrast to Nexus band structures in terms of their analyticity properties. We then discuss several Nexus band structures. Sec. \textsuperscript{IV} will finally give the method to state the band topology data in terms of homology classes of analytic loops on a generalized domain around the triple point. This won’t be hindered by a lack of gapped property, because analyticity near the degeneracies will constrain the wavefunctions enough to enable stating the topology. This will conclude our exposition on the band topology of Nexus fermions. We will end the paper in Sec. \textsuperscript{V} with an outlook towards the future and some open questions.

\section{2d ANALYTICITY}

In this section, we will start with the analyticity discussion in a 2d beyond-Dirac Nexus system. Let’s reconsider the band structure introduced in Ref.\textsuperscript{26} to set up the discussion:

\begin{equation}
H(p) = \begin{pmatrix}
0 & p_x - ip_y & p_z - ip_y \\
p_x + ip_y & 0 & p_z + ip_y \\
p_x - ip_y & p_z + ip_y & 0
\end{pmatrix}
\end{equation}

The eigensystem of $H(p)$ is

\begin{align}
\epsilon_\alpha(p) &= 2p_\alpha \cos \left( \frac{\theta_p}{3} + (2 + \alpha) \frac{2\pi}{3} \right) \\
v_\alpha(p) &= \frac{1}{\sqrt{3}} \left( \omega_\alpha^2 e^{-i\frac{2\pi}{3}} \left( \omega^* \right)^{2+\alpha} e^{i\frac{2\pi}{3}} 1 \right)^T \tag{2b}
\end{align}

where $\theta_p = \text{arctan} \left( \frac{p_y}{p_x} \right) \in [0, 2\pi)$. $\omega = e^{i\frac{2\pi}{3}}$, $\omega^2 = e^{-i\frac{2\pi}{3}}$ are the complex cube roots of unity and $\alpha = 0, 1, 2$. This band structure possesses a three-fold degeneracy at $p = 0$ clearly, and has two line degeneracies coming out from the triple point which is a signature feature of Nexus wavefunctions. Because of the line degeneracies, a standard Berry phase description of the wavefunction geometry is not applicable. However, we had used generalized winding numbers\textsuperscript{25,27} to understand this 2d wavefunction geometry (cf. Table I and Sec. II of Ref.\textsuperscript{29}) and contrasted with other known 2d Dirac-like wavefunction geometries. In 3d, such winding number description is 

not generally applicable for classification of point degeneracies. Thus, we will take the approach to be described below and in future sections.

Our main point of view will be to understand and write down the key aspects of the analytic behavior of various band structures. This is a different way of communicating invariant data of the wavefunction geometry than winding numbers and Berry phases. For example, we often view the familiar two-fold Dirac system

$$H_{\text{Dirac}}^K(p) = \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

(3)

with the eigensystem as

$$\epsilon_{\pm}(p) = \pm p; \quad v_{\pm}(p) = \frac{1}{i\sqrt{2}} (\pm e^{-i\theta} p, 1)^T$$

(4)

by calculating Berry phase or winding number on gapped region in one lower dimension (e.g. any closed loop around the degeneracy). We rather want to include the degeneracy to be a part of the analysis.

Firstly, on a gapped loop we clearly have the analyticity property

$$v_i(\theta + 2\pi) = v_i(\theta)$$

(5)

However, we also have the following analyticity property of Dirac wavefunctions

$$v_+(\theta + \pi) = v_-(\theta)$$

(6)

which connects the two bands. In fact, this relation tells us how to consistently arrive at the two-fold degeneracy from all sides without running into analytic ambiguities. Thus, we can interpret this as the way to move analytically across the point degeneracy. This is illustrated in the two figures from the left in Fig. 1.

**FIG. 1.** This figure illustrates the analytic way of moving across or through the Dirac point. The left and middle figures show how that analytic movement happens in the spectrum from the side and top views respectively. The right figure shows the analytic movement in the generalized domain. As mentioned in the text, the generalized domain is made of two copies of $p_x, p_y$ plane connected at the Dirac point. The color scheme is only for convenience.

Eq. 5 and 6 are nothing but an alternate way of describing the wavefunction geometry that is captured by Berry phase and winding numbers, with the additional benefit of allowing to move across the degeneracy in an analytically smooth way. This alternate viewpoint will prove useful for us because Nexus triple points can not be enclosed by a gapped region in one lower dimension. As notation, we refer to analyticity relations with the same band index on left and right hand sides as “index-preserving” (e.g. Eq. 5), while analyticity relations with different band indices on both sides as “index-connecting” (e.g. Eq. 6).

For a quadratic band touching (QBT), the analyticity relation is in fact

$$v_+(\theta + \pi) = v_-(\theta)$$

(7)

We can understand this in terms of two Dirac points (of same winding) sitting on top of each other. Let’s first imagine these two Dirac points are not on top of each other, and we move analytically across both the degeneracies in a single go. In this process, we will return back to the same band that we started from as illustrated in Fig. 2. Now, imagine moving these two Dirac points till they fall on top of each other to obtain a QBT. Analyticity thus forces us that we will stay in the same band when we cross the QBT (bottom panel of Fig. 2), i.e. Eq. 7. This argument also works when the QBT splits into more Dirac points, e.g. in Bernal-stacked honeycomb bilayer lattice in presence of “trigonal” warping terms when it splits into three Dirac points of same winding and a fourth one with opposite winding.28

With the above discussion in hand, we can revisit the 2d system in Eq. 1 and 2 in terms of its key analyticity information. The index-connecting relation is

$$v_i(\theta + 2\pi) = v_{i(\alpha + 1) \mod 3}(\theta)$$

(8)

which may be contrasted with Eq. 5 in the Dirac case. Similarly, in contrast to Eq. 6 in the Dirac case we arrive at the index-preserving relation

$$v_i(\theta + 6\pi) = v_i(\theta)$$

(9)
For Eq. 2 by re-writing as $\epsilon_R$iemann surfaces. This analogy can be made exact as expressed through band-indexed eigenfunctions in analogy with the wavefunction geometry. We can imagine a single Dirac touching and a QBT differ in their analytic movements across the degenerate point.

This unusual “$+6\pi$” structure is a result of the Nexus lines emanating from the three-fold degeneracy. We emphasize that the above two relations are an alternate way of stating the wavefunction geometry via the analyticity

The band-connection relation (Eq. 6) gives us the rule of moving through the “connecting point” in the generalized domain from one copy of the $p_x-p_y$ plane to the other (see the rightmost figure of Fig. 1). In the Dirac case, there is no branch cut structure since the eigensystem (Eq. 4) is perfectly analytic. The generalized domain will be used when we discuss the 3$d$ Nexus wavefunctions in the next sections.

III. 3$d$ ANALYTICITY

In this section, we start with the actual discussion on the analyticity properties of 3$d$ Nexus fermions. As mentioned in Sec. I, line degeneracies are exceptional in 3$d$ and require symmetry protection, whereas they are fine-tuned in 2$d$. Thus the analyticity discussion in the previous section is for a fine-tuned case, but it will help us in the following discussions. Before we go towards Nexus analyticity properties, let us start with the familiar case of Weyl point degeneracies to set the stage.

A. Weyl analyticity

A Weyl point degeneracy is characterized by an effective (low-energy) Hamiltonian of the form $H^{\text{Weyl}} = \sum_{i \in \{x,y,z\}} p_i \sigma_i$. The eigenenergies are $\epsilon(p) = \pm p$, and the eigenfunctions are generally expressed as

\[
v_+(p) = \left(e^{-i\phi} \cos(\theta/2) \sin(\theta/2)\right)^T, \quad v_-(p) = \left(-\sin(\theta/2) \ e^{i\phi} \cos(\theta/2)\right)^T.
\]

In our gauge choice where the last term is kept purely real, they are

\[
v_+(p) = \left(e^{-i\phi} \cos(\theta/2) \sin(\theta/2)\right)^T, \quad v_-(p) = \left(-e^{-i\phi} \sin(\theta/2) \cos(\theta/2)\right)^T.
\]

Often, the wavefunction geometry of 3$d$ point degeneracies are understood by considering a 2$d$ surface enclosing the point degeneracy and computing the Chern number of the two gapped bands on this reduced 2$d$ system. For the Weyl system, the Chern number of the two gapped bands are $\pm 1$. We note that in the full BZ, the number of Weyl points has to be even such that the sum of their Chern numbers is zero, as the Chern number computed on the BZ boundary must be zero by periodicity.
Another perspective on the Weyl geometry is the following: consider 2d cross-sections in the Brillouin zone away from the point degeneracy, e.g., a constant $k_z$ plane which is a representative 2d system. In such cross-sections, we obtain a gapped Dirac cone system with the specific sign of the mass term controlled by the sign of $p_z$. Because the 2d system is gapped, we may compute a Chern number. On either side of the Weyl point, the sign of the mass changes. Thus, the Weyl degeneracy may be interpreted as a transition between the two topologically different 2d Chern bands on either side.

However, anticipating the lack of gapped 2d surfaces in presence of line degeneracies for Nexus fermions, we may ask what happens if we were to consider cross-sections which always include the Weyl point, e.g., consider any plane going through the Weyl point. In particular, if we consider a family of such planes -- e.g. all planes containing $p_z$-axis --, then we would like to ask how does this family of 2d bands interpolate among each other? This forces us to grapple with the role of the degeneracy in the analysis. This is a similar motivation to what we have done in 2d as in Sec. II where stating the index-connection relation is our way of answering this question. In 3d we will need to make a choice of the coordinate system, however for the Weyl discussion, the spherical symmetry comes to our rescue and we can use the $p_z$ axis to set up our spherical coordinates without any loss of generality. The analyticity relations are the following:

\begin{align}
  v_+(\pi - \theta, \phi + \pi) &= v_-(\theta, \phi) \quad (12a) \\
  v_i(\theta, \phi + 2\pi) &= v_i(\theta, \phi). \quad (12b)
\end{align}

Graphically speaking, we have to exit in the same “direction” that we came in towards the degeneracy. This is the exact same behavior as shown in Fig. 1 in one higher dimension. We notice here that Eq. 12a conveys the same information as the changing sign of mass in a different way. Finally, the generalized domain restatement will now consist of two copies of the $p_x$-$p_y$-$p_z$ space joined again at the point degeneracy with the above analyticity relations (Eq. 12a 12b) as the rules to move in this generalized domain.

### B. Nexus analyticity

Now, we tackle the main case of 3d Nexus triple points. Using $SU(3)$ generators $\Lambda^i$ (the Gell-Mann matrices) for brevity, the 2d Nexus system (Eq. 7) looks like

\[ H(p) = p_x(\Lambda^1 + \Lambda^4 + \Lambda^6) + p_y(\Lambda^2 + \Lambda^5 - \Lambda^7). \quad (13) \]

To this, we start by adding a diagonal $\Lambda^3$ “mass” term linear in $p_z$ (in analogy with $p_x \sigma_z$ for the Weyl case) such that we get a 3d Nexus triple point. Thus we have

\[ H^3(p) = H(p) + p_z \Lambda^3 \quad (14) \]

**Fig. 3** shows the line-degeneracy structure and the triple point given by Eq. 14.

Similar to the Weyl discussion, we will discuss 1) how do the (generic) 2d cross-sections away from the triple point evolve as we cross the triple point and 2) what are the analyticity relations that characterize the presence of triple points. We will sometimes refer to them as topological defects or monopoles in analogy with Weyl point degeneracies (Sec. IV will give a topological classification of these defects). Also, line degeneracies are extended topological defects present in the Nexus system. Ref. gave a $Z_2$ topological charge to the line degeneracy by computing a $Z_2$ topological invariant (cf. Eq. 1 on a $d - 2 = 1$ dimensional loop around the line degeneracy. One can also compute a winding number on such loops which is a $Z$ invariant.

The eigensystem formula for $H^3$ is comparatively in-
volved than Weyl eigensystem (Eq. 11) and we do not write it down explicitly. The exact details are not relevant to understand the analyticity properties. Fig. 3 shows the evolution of (generic) 2d cuts across the triple point. We see that on one side the top and middle bands are joined by a Dirac point with the bottom band as standalone, while on the other side the bottom and middle bands are joined by a Dirac point with the top band as standalone. The triple point is thus to be thought as a defect which separates these two different behaviors. We can think of these behaviors as two different $SU(2)$ groups, one involving middle and top bands and another involving middle and bottom bands. In comparison to the Weyl degeneracy, where the sign of the Dirac mass changes on either side, here the triple point degeneracy is changing one type of $SU(2)$ defect to the other type.

To write down the analyticity relations for the $H^3$ triple point, we will again be motivated by how the family of 2d systems on cross-sections that include the triple point interpolate among each other. There are two such examples one shown in Fig. 3 and another shown in Fig. 4. We see that certain cross-sections will resemble the 2d Nexus system (as in Fig. 3), while certain cross-sections will resemble a $SU(2)$ spin-1 system (as in Fig. 3).

For the 2d Nexus-like cross-sections, the analyticity relations are given by Eq. 8 (and 9). While for the 2d spin-1 cross-sections, they are

\[
\begin{align*}
v_{\text{top}}(\theta + \pi) &= v_{\text{bottom}}(\theta) \\
v_{\text{middle}}(\theta + \pi) &= v_{\text{middle}}(\theta).
\end{align*}
\]

and clearly also the relation $v_i(\theta + 2\pi) = v_i(\theta)$. We note here that Eq. 15b captures the spin-1 nature as opposed to a two-fold Dirac degeneracy and a third standalone band.

To give a different example, we quickly look at the case of adding a diagonal $A^8$ “mass” term

\[
H^8(p) = H(p) + p_z A^8
\]

For this case, there is line degeneracy along $p_x$-axis as well as $p_z$-axis connected to the triple point degeneracy. (One can easily see the $p_z$-axis degeneracy coming from the eigenspectrum of $H^8(p_x = 0, p_y = 0, p_z)$. This is illustrated in the top panel of Fig. 5). Generic cross-sections for $H^8(p)$ will contain two Dirac points either on the same pair of bands, or on different pairs of bands always involving the middle band. We can again define analyticity relations similar to Eqs. 8, 9, 15 for corresponding cross-sections containing the triple point.

Finally, we end this section with the generalized domain restatement for the 3d Nexus systems discussed above. It will consist of three copies of $p_x - p_y - p_z$ space which are joined appropriately at the line degeneracies (for both $H^3$ and $H^8$) and the triple point, with the above analyticity relations giving us unambiguous rules to move in this generalized domain. In the next section – where we build a classification scheme for Nexus triple points – we will restrict ourselves to a $d - 1 = 2$ dimensional closed surface enclosing the triple point as is done for the Weyl case. Again the analyticity relations will come to our aid to govern how to move smoothly in this (generalized) 2d surface.

\section{IV. Classification}

In the previous sections, we established the rules to move smoothly in our parameter space. Here, parameter space refers to the generalized domain. In this section, we will describe a (topological) classification scheme for different kinds of Nexus triple points by making use of these rules. Given a Nexus system, the basic idea will be to consider an enclosing surface around the triple point in the generalized domain. As remarked at the end of the previous section, the enclosing surface in the generalized domain consists of three copies of the surface (e.g. spheres) joined at the points where the line degeneracies cross them. On this generalized enclosing surface, we will categorize the various topologically distinct ways in which one may analytically loop back to the start point. This is reminiscent of the concept of homology classes.
of 1-cycles in topological classification of geometric objects. A very familiar example of this are the non-trivial loops that one draws on a torus that can not be shrunk to a point, whereas on a sphere there are no such loops. Importantly, the analyticity relations discussed before allows us to focus only on the enclosing surface to capture the topological data of the wavefunction geometry without the full knowledge of the wavefunctions themselves.

Let's start with $H^8$ in this case. The enclosing surface for this is shown in Fig. 5. Let us imagine drawing topologically distinct loops on this. Clearly there exist (trivial) loops that can be shrunk to a point (not shown in the figures). $H^8$ also hosts non-trivial loops which are shown in Fig. 6. We see there are two kinds of loops:

1. those that straddle different spheres. The drawing of such loops relies on the index-connecting kind of analytic relations.

Close to the connecting point on the 2$d$ enclosing surface, we can imagine a small flat coordinate patch giving us our local coordinate system in which we may use Eq. 6. Therefore, in the drawing of the loop through the connecting point, we have to use the step illustrated in Fig 4. A corollary is that there can not be a non-trivial loop on a single sphere that touches the Dirac-like connecting point.

With these basic steps in hand, we can enumerate all the non-trivial homological classes and they are shown in Fig. 6. There are three categories of non-trivial loops. They are

2. loops involving only two connecting points, they can be either on the left-middle sphere pair, or middle-right sphere pair.

2. Loops involving all the connecting points, the two connecting points on the left and right spheres have
FIG. 7. The top panel shows the enclosing surface in the original domain. In the generalized domain, the corresponding enclosing surface consists of three connected spheres with associated connecting points as shown in the second panel. There is only one non-contractible loop one that can be drawn in the middle sphere. Any loop on the left and right spheres can be contracted to a point. On the non-contractible loop, one can calculate the Berry phase which will turn out be $\pm \pi$.

3. Loops on the same sphere that enclose the connecting points.

For the case of $H^3$, the generalized enclosing surface is shown in second panel of Fig. 7. For this case there is only one possible non-contractible loop in the middle sphere. This captures the band topology of $H^3$ and shows its distinction from $H^8$ (and other cases). From the above discussions, we can immediately conclude that the $\Lambda^8$ triple point and two different $\Lambda^3$ and $\tilde{\Lambda}^3$ triple points inside the enclosing surface are not topologically different.

In our scheme, the distinction between different topological cases are categorized using the non-contractible loops or 1-cycles. The number of distinct loops only depends on the number (and kind) of the connecting points (Dirac-like, or possibly QBT as in the examples to follow) on the enclosing surface. Thus one cannot distinguish between pair of $\Lambda^3$, $\tilde{\Lambda}^3$ triple points and a single $\Lambda^8$ triple point which gives us a thumb rule for composition of these triple point topological defects.

We end with an application of our scheme to recent Nexus triple points discussed in the literature which have possible material realizations. For the type II nexus system as notated by Chang et al., there are four line degeneracies coming out of the triple point: one along the $z$-axis and the rest three oriented at $\frac{2\pi}{3}$ angular separation about the $z$-axis lying in high symmetry planes. See Eq. 2,3 in Ref.13 for the low-energy Hamiltonian, and Fig. 1 for the line degeneracy structure. This happens due to the $C_{3z}$ symmetry. In this case, the generalized domain for the surface enclosing the triple point degeneracy will have three spheres connected to each other at the points where they intersect the line degeneracies. The topology of this system can thus be similarly understood using the homology classes as discussed above. On this surface the loops are again of three main types (diagram not show due to proliferation of non-contractible loops): 1) loop enclosing one connecting point, 2) loop spanning two spheres, 3) loop spanning through 3 spheres. Even though these three types were also present in the case of $H^8$, the count of each type is different which topologically distinguishes the two cases.

The case of type I as notated by Chang et al is worth noting. The generalized enclosing surface in this case looks similar to that of $H^3$ (Fig. 7). However, the classification of non-contractible loops is different than the $H^3$ case. This is due to the degeneracies being QBT-like in this case. Thus while drawing the loops, we have to follow the rule as shown in Fig. 2's bottom panel. This allows for a new kind of non-contractible loop on the same sphere which goes through the connecting point. We show the various possible loops in Fig. 8. This new kind of loops as in middle and bottom panel of Fig. 8 are not possible when the connecting points are Dirac-like because in that case we are necessarily forced to go to the connected sphere due to analyticity (Fig. 1). We remark here that Ref. 13's statement that the line degeneracies
are characterized by a $2\pi$ Berry phase does not paint the full picture. Such a characterization strictly can only be applied to the non-contractible loop shown on the top panel of Fig. 3 and not in general. Our scheme helps to make clear which loops have a topological property based on analyticity. Once we have such loops in hand, we may compute familiar topological invariants\textsuperscript{14} on the gapped ones among them.

### V. CONCLUSIONS

In summary, we laid a general scheme to describe the band topology of the so-called Nexus triple point fermions. This was based on an understanding of the analyticity properties near (line-)degeneracies which are an integral part of the Nexus band structure. This scheme is built on the insight gained in Ref\textsuperscript{22} where we could see the analyticity properties near a line degeneracy explicitly. The discussion started with the known cases of Dirac and QBT bands in 2d in Sec. II. We use analyticity to define a generalized domain where we go smoothly across the “connecting” points at the degeneracies (see Fig. 1). We emphasise that in the original domain there is a non-analyticity in the space of wavefunctions at a (non-accidental) degeneracy which is then considered as a topological defect. In the generalized domain, however this issue is not there. For the 2d Nexus case, the generalized domain is a familiar object – Riemann surfaces associated with $z^{1/3}$ – known from the study of complex analysis. However the general idea will be applicable in any situation. So we take this scheme to 3d and define generalized domains for 3d Nexus triple points in Sec. III.

In analogy with Weyl points and Chern numbers on associated enclosing surfaces, we characterize the 3d Nexus points by enclosing them in the generalized domain (see bottom panel of Fig. 3-7) in a departure from existing literature. Sec. IV describes the triple point defect topology in terms of non-contractible loops that can be drawn on this enclosing surface. These are the 1-cycle homology classes of the generalized domain. Different Nexus triple points have their unique data of these 1-cycle homology classes. This discrete set of data gives the triple point its topological character, since they will be stable to small deformations of the Hamiltonian. We emphasize here again that this description characterizes the Nexus triple points themselves. Line-degeneracies on the other hand are characterizeable by using topological invariants defined on the gapped loops around them\textsuperscript{10}. Our enclosing scheme is finally applied to an example of Nexus triple point in the literature which has a possible material realization\textsuperscript{10} whereas only the topology of gapped enclosing loops around the line degeneracies and their evolution across the triple point had previously been discussed\textsuperscript{11,13,24}.

This final result of our paper provides a general answer to the question of Fermi arc protection in Nexus systems that was raised by Ref.\textsuperscript{15} Since the Nexus triple points are topological in nature, therefore the associated surface arcs will be protected and will necessarily go through the projections of the Nexus triple point. The details of this process is an interesting topic for further study with some speculative thoughts presented at the end.

We end with some discussion on the conceptual issues that still remain to be understood. One thing that we have puzzled over is that if there exits a Chern number like description of the Nexus triple point topology by making use of the Berry connection/curvature technology, in spite of the absence of a gapped enclosing surface which motivated the entire line of reasoning in this paper. Instead of thinking as a single analytic “band” defined on the generalized domain which gave us our homological classification scheme, if we think of three bands on the conventional domain then the Dirac points are like monopoles on the enclosing surface. The associated Berry curvature will thus diverge at the degeneracy points on the sphere. So the integral of the Berry curvature over the sphere is not guaranteed to be well-defined. Could there still be a finite piece in this integral which might capture the underlying topological nature?

Another approach could instead be to consider a non-Abelian characterization. In fact, this approach can be implemented for the 2d example $H$ introduced in Sec. II. A similar implementation in 3d is not yet clear to us, but we may anticipate a matrix of topological charges instead of a single scalar charge. Finally, some other mathematical machinery might be useful that we don’t anticipate yet.

We end with some final thoughts on connecting to possible experimental observables. As mentioned before, the topological character of degeneracies in the bulk have profound effects on the surface states, e.g fermi-arcs in Weyl semimetals.\textsuperscript{19} Thus for the case of the Nexus triple point, we may specifically ask how the homological loop classes identified in this paper – especially the ones which live on multiple spheres – affect the surface states. Each homological class may leave its own distinct imprint on the surface states which can perhaps be identified in experiments or simulations. Of course, the effect of electron-electron interactions\textsuperscript{37} or disorder on Nexus systems are yet to be fully explored.

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