Knotted Non-Hermitian Metals

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We demonstrate that knotted metallic band structures occur as a new form of stable topological phases in non-Hermitian (NH) systems. These knotted NH metals are characterized by open Fermi surfaces, known in mathematics as Seifert surfaces, that are bounded by knotted lines of exceptional points. Quite remarkably, and in contrast to the situation in Hermitian systems, no fine tuning or symmetries are required in order to stabilize these exotic phases of matter. By explicit construction, we derive microscopic tight-binding models hosting knotted NH metals with strictly short-ranged hopping, and investigate the stability of their topological properties against perturbations. Building up on recently developed experimental techniques for the realization of NH band structures, we discuss how the proposed models may be experimentally implemented in photonic systems.

Introduction.— Revealing the topological properties of Bloch bands has revolutionized the theory of solids: Fascinating new forms of quantum matter such as topological insulators [1, 2] and Weyl semimetals [3] have been discovered and theoretically described in terms of topological invariants that measure how the phase of the Bloch functions twists in reciprocal space [4]. Recently, the experimental discovery of topological phases in various dissipative systems subject to gain and loss [5–13] has triggered the urgent quest for generalizing this topological band theory to non-Hermitian (NH) systems [14–43]. While a comprehensive understanding of the role of topology in NH systems is still lacking, several crucial differences to the Hermitian realm have already been established. Prominent examples of these include a modified relation between bulk topological invariants and protected surface states (bulk boundary correspondence) [16–18] as well as qualitative changes in the topological stability of nodal surfaces [19–23]. Regarding the latter, extending the notion of band touching points to that of exceptional points (EPs) in NH systems, leads to the occurrence of nodal band structures in lower spatial dimensions [20, 44], where conventional band touching points would be unstable, or dependent on symmetries [45, 46].

Drawing intuition from this fundamental observation, here we show and exemplify how topologically stable nodal lines can naturally form knots in reciprocal space in three-dimensional (3D) NH systems (see Fig. 1 for an illustration), thus introducing a new form of metallic NH topological phases. Remarkably, these knotted lines of EPs necessarily bound open Fermi surfaces, known in mathematics as Seifert surfaces, the topological properties of which are closely related to a knot invariant characterizing the nodal line. This general approach is illustrated by the explicit construction of microscopic tight-binding models with strictly short-ranged hopping that realize paradigmatic examples of knots such as the trefoil knot shown in Fig. 1. Furthermore, we investigate the stability of the knotted nodal lines against perturbations, and discuss platforms for the experimental realization of knotted non-Hermitian metals.

Knotted exceptional lines and open Fermi surfaces.— An interaction free system with two bands is fully characterized in reciprocal space by its Bloch Hamiltonian which may be written as

\[ H(k) = \mathbf{d}_R(k) \cdot \mathbf{\sigma} + i \mathbf{d}_I(k) \cdot \mathbf{\sigma}, \]  \hspace{1cm} (1)

where \( \mathbf{k} \) denotes the lattice momentum, \( \mathbf{\sigma} = (\sigma_x, \sigma_y, \sigma_z) \), and \( \mathbf{d}_R, \mathbf{d}_I \in \mathbb{R}^3 \). Nodal points then correspond to coalescence of the eigenvalues

\[ E^2(k) = d_R^2(k) - d_I^2(k) + 2id_R(k) \cdot d_I(k) \]  \hspace{1cm} (2)

which is satisfied when both

\[ \text{Re}[E^2] = d_R^2 - d_I^2 = 0 \]  \hspace{1cm} (3)

Figure 1. Illustration of a knotted nodal band structure obtained from a tight-binding model with a hopping range of two lattice constants defined by Eqs. (8,17) with \( \Lambda = -20 \). The solid blue line is a trefoil knot corresponding to the exceptional lines of the model that correspond to the intersection of the surfaces \( \text{Re}[E^2] = 0 \) and \( \text{Im}[E^2] = 0 \) which are marked red and green respectively in (a). (b) Shows the same exceptional knot (blue) and its concomitant open \( \text{Re}[E] = 0 \) Fermi surface (green). This trefoil knot is also called the \((3, 2)\) torus knot and is the most elementary representative of the general family of \((p, q)\) exceptional torus knots constructed in this work.
and
\[ \text{Im}[E^2] = 2d_R \cdot d_f = 0. \]  

We stress that these solutions generally correspond to exceptional points where the Hamiltonian becomes defective, i.e. non-diagonalizable with only a single eigenvector associated with the two-fold degenerate eigenvalue [47]. It is only for the trivial solution \( d_R(k) = d_f(k) = 0 \) of Eqs. (3,4) that the nodal points are of the conventional type encountered in Hermitian systems.

In three dimensions, the solutions to Eq. (3) and Eq. (4) each describe closed surfaces, with intersections in the form of closed lines. These are in turn connected by open Fermi surfaces [20], as follows from the eigenvalue equation (2): Requiring Re \( E \) = 0, we find
\[ \text{Im}[E^2] = 0, \quad \text{Re}[E^2] \leq 0, \]  

implying that the Fermi surface Re \( E \) = 0 is a subset of the closed surface Im \( E^2 \) = 0, and is as such generally open. Similarly, we can define an open i-Fermi surface by requiring Im \( E \) = 0 which leads to the conditions
\[ \text{Im}[E^2] = 0, \quad \text{Re}[E^2] \geq 0. \]  

If a particle-hole symmetry breaking term \( d_0(k) \) is added to the Hamiltonian, then the Fermi (i-Fermi) surfaces simply inherit this shift but are still described by a vanishing real (imaginary) part of the band splitting. Thus, if there are defectivities in the spectrum, there is always a corresponding Fermi surface (or nodal surface) which is necessarily open and terminates on the exceptional lines. This close connection between band touching points and the Fermi surfaces is manifested in the emergence of Fermi ribbons in systems where the nodal topology exhibits a nontrivial linking number [20].

The insight that exceptional lines occur at the intersections of orientable surfaces forming the solutions of Eqs. (3,4) provides a natural starting point for generating non-Hermitian models with topologically non-trivial nodal lines in a constructive and systematic fashion, for example by means of the following construction. We start by considering two surfaces \( s_1 \) and \( s_2 \) in momentum space with a topologically nontrivial intersection. Next, we assume two real and continuous scalar functions \( f_1 \) and \( f_2 \) that vanish on these surfaces, i.e.
\[ f_i(k \in s_i) = 0, \quad i = 1, 2. \]  

Then we may encode the topology of the intersection of \( s_1 \) and \( s_2 \) into our model Hamiltonian by taking
\[ d_R(k) = (f_1(k) - \Lambda, \Lambda, 0), \quad d_f(k) = (0, f_2(k), \sqrt{2}\Lambda) \]  

which, using Eqs. (3,4), gives
\[ \text{Re}[E^2] = f_1^2 - f_2^2 - 2f_1\Lambda, \quad \text{Im}[E^2] = 2f_2\Lambda. \]  

In the limit of \( \Lambda \to \pm \infty \), we obtain solutions to Eq. (3,4) exactly at the intersection \( s_1 \cap s_2 \), where changing the sign of \( \Lambda \) results in an interchange of the Fermi and i-Fermi surfaces respectively. Finite values of \( |\Lambda| \) lead to deformation of the surfaces Re \( E^2 \) = 0, Im \( E^2 \) = 0, according to Eq. (9). Thus, given a sufficiently large magnitude of \( \Lambda \), the nodes of the model Eq. (8) will inherit the topology of \( s_1 \cap s_2 \). Furthermore, since the nodes occur at finite \( d_R, d_f \), they are necessarily exceptional, i.e. they correspond to defective lines of the Hamiltonian.

To generate the functions \( f_1, f_2 \) such that the intersection of \( s_1 \) and \( s_2 \) obtains a nontrivial topology, we note that a torus knot or link may be described as the solution to a complex algebraic equation on the unit three-sphere. Specifically, consider a pair of complex scalars \( (Z_0, Z_1) \subset \mathbb{C}^2 \) and a corresponding unit three-sphere \( S^3 \) given by
\[ |Z_0|^2 + |Z_1|^2 = 1. \]  

The \((p, q)\) torus knot or link is then described by the solution to
\[ g(Z_0, Z_1) = Z_0^p + Z_1^q = 0 \]  

on \( S^3 \), i.e. subject to the constraint in Eq. (10). To generate knots in the band structure, we then map the momentum space onto the three-sphere so that, \( Z_0, Z_1 \) obtain an explicit \( k \)–dependence that satisfies Eq. (10). While there exist many ways to achieve this, here we follow the construction outlined in Ref. 48 (see supplementary material for technical details about the construction of knots and links [49]).

Having connected \( g(Z_0, Z_1) \) to the momentum space we note that it can be parameterized in terms of two real scalar functions by defining [53]
\[ f_1(k) + if_2(k) = g(Z_0(k), Z_1(k)). \]  

Then, according to Eq. (11), the functions \( f_1, f_2 \) satisfy Eq. (7), with \( s_1, s_2 \) being orientable surfaces such that their intersection \( s_1 \cap s_2 \) describes a \((p, q)\) knot or link. Furthermore, according to Eqs. (5) and (9) the Fermi surface is now a subset of \( s_2 \).

A few examples of nodal topologies generated from this procedure are displayed in Fig. 2. Here, for the exceptional lines to form torus knots, we stress that \((p, q)\) need to be chosen as coprime. Otherwise, Eq. (12) produces links rather than single knots.

It is worthwhile to note that it is not possible to uniquely determine the topology of the Fermi surface solely from the knot, even though certain generic conclusions can be drawn. The genus of a knot is defined as the minimal genus of a Seifert surface whose boundary it forms [50]. Thus, given the genus of a torus knot
\[ G_{\text{knot}} = (p-1)(q-1)/2, \]  

we obtain a lower bound for the genus of the Fermi surface, or indeed the i-Fermi surface
\[ G_{\text{Fermi}} \geq (p-1)(q-1)/2. \]

This result corresponds to the intuition that the topology of the Fermi surface (i-Fermi surface) can acquire additional
handles, hence increasing its genus, without altering its open boundary given by the exceptional knot.

**Knotted tight-binding models.**—To realize exceptional knots in explicit lattice models using the methods described above, it is clear that the mapping from \( k \)-space now should connect the three-sphere with the Brillouin zone rather than \( \mathbb{R}^3 \). However, a key point to note at this stage is that knots may in principle be parameterized equally well on highly deformed three-spheres as long as their topology remains intact. This fact may be exploited to obtain a mapping where \( Z_0, Z_1 \) are linear functions of short-range hoppings, which in turn translates to a simpler tight-binding model. Here, we thus use a construction of the form

\[
Z_0(k) = \sin k_x + i \sin k_y,
\]

\[
Z_1(k) = 2 \sum_{\alpha} \cos k_{\alpha} - 5 + i \sin k_z,
\]  

(15)

where \( f_1, f_2 \) are as before given by Eqs. (11) and (12). As an example, we consider the trefoil knot corresponding to \((p, q) = (3, 2)\), which represents the simplest torus knot and is described by

\[
f_1(k) + i f_2(k) = Z_0^0(k) + Z_1^1(k).
\]  

(16)

The highest order terms, and thus the most long-ranged dispersion results from the third order terms \( \sim \sin^3 \) in \( Z_0^3 \). Introducing the approximation \( \sin^2 x \approx 2 - 2 \cos x \), which is correct up to \( O(x^4) \), the resulting theory contains terms up to quadratic order, implying that the range of the hopping is now two unit cells. The explicit form of \( f_1, f_2 \) is then given by

\[
f_1 = 30.5 - 20 \sum_\alpha \cos k_{\alpha} + 2 \sum_\alpha \cos 2 k_{\alpha} + \frac{1}{2} \cos 2 k_z
\]

\[+ 4 \sum_{\alpha \beta} \cos (k_{\alpha} \pm k_{\beta}) + 3 \sin k_x \pm k_y - 2 k_x - 4 \sin k_z
\]

\[
f_2 = 4 \sin k_y - 10 \sin k_z + 2 \sin k_y + 2 \sin 2 k_z
\]

\[+ 3 \sin (k_x \pm k_y) \pm 2 \sin (k_y \pm k_z) \pm 2 \sin (k_z \pm k_x),
\]  

(17)

where \( \pm \) denotes a summation over \((-1, 1)\). Albeit somewhat complex in structure it is worth noting that the hopping amplitudes decay rapidly with distance and are smallest for the longest range hopping of two lattice constants. The corresponding tight-binding model, which results from inserting Eq. (17) into Eq. (8) with \( \Lambda = -20 \), is displayed in Fig. 1.

Proceeding to knots of higher genus, the complexity of the lattice models naturally increases. To obtain the \((5, 2)\) and \((5, 3)\) nodal structures displayed in Fig. (2, a and b), we must include terms \( \sim Z_0^5 \). Exploiting trigonometric identities and approximations as above, it is possible to arrive at a description where the range of hopping is up to three unit cells.

We note that if \((p, q)\) are both even, there is a much simpler way to encode them into a nodal structure than the generic construction given by Eqs. (8,11), by instead taking

\[
H = Z_0^{p/2}(k) \sigma_i + Z_1^{q/2}(k) \sigma_j, \ i \neq j,
\]  

(18)

which gives exceptional nodes described by

\[
E^2 = Z_0^p(k) + Z_1^q(k) = 0,
\]  

(19)

immediately reproducing Eq. (11). A key advantage of using this additional structure is that the resulting tight-binding models become both simpler and shorter ranged. For example, the Hopf link given by \((p, q) = (2, 2)\) can be obtained already from nearest neighbor hopping by using the map (15), see Fig. 3. However, to obtain knots rather than links, we stress that it is necessary that \((p, q)\) are coprime integers.

**Stability.**—We emphasize that nodal lines, knots or links in non-Hermitian systems differ fundamentally from their Hermitian counterparts in the sense that their realization or stability does not depend on the existence of symmetries or fine-tuning. This circumstance is manifested in the fact that band touching points are described by only two equations (3,4) so that they generically become line-like in three spatial dimensions. Correspondingly, the nodal knots that we discuss here are stable in the sense that their topology cannot be altered by any deformation until the point where reconnections or crossings of exceptional lines occur, or where their size is shrunk to zero. Thus, introducing perturbations to the Hamiltonian of the form

\[
H(k) \rightarrow H(k) + \sum_{i=x,y,z} \delta_i \sigma_i, \ \delta_i \in \mathbb{R}
\]  

(20)
we obtain a finite range of perturbations \( |\delta_i| \) in which the nodal topology remains intact. We note that similar arguments hold for anti-Hermitian perturbations, upon multiplying the entire Hamiltonian by the imaginary \( i \).

On a quantitative note, for the trefoil knot described by Eq. (17) with \( \Lambda = -20 \), we find that the critical magnitudes \( |\delta_i^c| \) of perturbations are anisotropic, but all fall into the range \( 0.4 < |\delta_i^c| < 0.7 \). Comparing to (17), we infer that this corresponds to \( 4 - 7\% \) of the largest nearest neighbor hopping integral.

For the Hopf link shown in Fig. 3, the perturbations required to alter the nodal topology fall into the range \( 0.85 < |\delta_i| < 2.75 \). Comparing this to Eq. (15,18), we find that the perturbation required to dismantle the link generally needs to be at least of the same order of magnitude as the hopping integral. Thus, this construction is not only very simple, with hopping terms of only one unit cell, it also features a remarkably high stability towards perturbations.

**Experimental realization.**—There are several physical settings that have the potential to host knotted non-Hermitian metals, including photonic and acoustic metamaterials, cold atoms [22], and even strongly disordered and interacting materials [25, 41, 42]. Each of these prominently feature disipation which is a prerequisite for an effective non-Hermitian description and especially the artificial systems enjoy a high degree of tunability by design. In particular, photonic systems [51, 52], where the photonic band structure can be directly probed by scattering experiments, are promising due to their high degree of control, especially in the light of the very recent experimental realization of both bulk Fermi arcs [5] in two-dimensional systems and exceptional rings in three dimensions [9].

Regarding the specific ingredients of our model, we note that the required large anti-Hermitian component \( d_{1,2} \) in Eq. (8) needed in our construction of exceptional knots is straightforwardly implemented via a staggered loss (and/or gain) profile within the unit cell [8, 10]. While asymmetric hopping corresponding to \( d_{1,2} \) is more demanding, such terms have also been experimentally realized [12, 13]. Thus, although the realization of the tight-binding models that we propose is certainly demanding, given the required control over hopping parameters with a range of two unit cells, all the basic ingredients for realizing knotted non-Hermitian metals are already available. As a precursor of single knots, at least the experimental realization of NH nodal links becomes an immediately experimentally feasible milestone due to our simplified construction (18). There, in contrast to previous work on corresponding Hermitian systems [53–55], only nearest neighbor hopping is required, and the resulting tight-binding model is extremely stable against generic perturbations.

**Discussion.**—In this work we have introduced the notion of knotted non-Hermitian metals as a new class of topological phases of matter. Remarkably, despite their apparent complexity, we have shown by explicit construction that non-trivial examples of knotted NH metals can be robustly realized in quite simple tight-binding models.

To clarify in what sense our findings conceptually go beyond the Hermitian realm, we would like to emphasize two crucial differences to the recently studied nodal knots in Hermitian systems [53]. First, simple parameter counting shows that in Hermitian systems, the occurrence of nodal lines requires fine-tuning or the presence of symmetries, since there only isolated nodal points are generically stable. By contrast, the NH nodal knots discussed in our present work are stable to any small perturbation. Second, the protected open Fermi surfaces occurring in the intriguing form of Seifert surfaces in knotted NH metals are a direct consequence of the fact that we consider knots of exceptional lines rather than ordinary (Hermitian) nodal lines. The non-diagonalizability of such NH knots thus necessarily leads to topological metals, while nodal knots in symmetry preserving Hermitian systems entail semimetals.

In a broader context, a deep connection between knot theory and topological quantum field theories in (2+1)D was first revealed in a seminal paper by Witten [56]. Later on, the theory of topological Bloch bands has been viewed as a non-interacting special case of such topological quantum field theories [57]. Our present analysis of non-Hermitian systems reveals another aspect to the role of knots in the topological classification of matter, where metallic non-Hermitian band structures are directly distinguished by the knot invariants associated with their open Fermi surfaces.

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