Knots and Non-Hermitian Bloch Bands

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Knots have a twisted history in quantum physics. They were abandoned as failed models of atoms. Only much later was the connection between knot invariants and Wilson loops in topological quantum field theory discovered. Here we show that knots tied by the eigenenergy strings provide a complete topological classification of one-dimensional non-Hermitian (NH) Hamiltonians with separable bands. A $\mathbb{Z}_2$ knot invariant, the global bioriented Berry phase $Q$ as the sum of the Wilson loop eigenphases, is proved to be equal to the permutation parity of the NH bands. We show the transition between two phases characterized by distinct knots occur through exceptional points and come in two types. We further develop an algorithm to construct the corresponding tight-binding NH Hamiltonian for any desired knot, and propose a scheme to probe the knot structure via quantum quench. The theory and algorithm are demonstrated by model Hamiltonians that feature for example the Hopf link, the trefoil knot, the figure-8 knot and the Whitehead link.

Extending topological band theory to non-Hermitian (NH) systems has significantly broadened and deepened our understanding about the topology of Bloch bands. NH Hamiltonians [1–6] are effective descriptions of a diverse set of many-body systems ranging from photonic systems with gain or loss [7–28] to quasiparticles of finite lifetime [29–36]. In contrast to Hermitian NH Hamiltonians have complex eigenenergies. This unique property gives rise to a number of intricate phenomena without Hermitian counterparts including for example the exceptional point (EP), where eigenstates coalesce [37–39], and the NH skin effect [40–54], where an extensive number of eigenmodes are localized at the boundary. A synopsis of earlier NH band theory is the classification of topologically distinct NH Hamiltonians based on symmetry [55–60] akin to the Hermitian ten-fold way [61–64]. This classification scheme starts by distinguishing two types of band gaps, the line gap and point gap. While NH bands with line gaps can be continuously deformed to their Hermitian counterparts, the point-gap topology is intrinsically NH [65–68] and explains the NH skin effect.

Recently it was recognized that the NH band theory in Refs. [55–58] based on the gap dichotomy is incomplete. A NH Hamiltonian may not possess a well-defined point or line gap. A more general theory only assumes separable bands [69], i.e. the eigenenergies $E_j(k) \neq E_l(k)$ for all $j \neq l$ and crystal momentum $k$. Moreover the ubiquitous twisting and braiding of complex eigenenergies give rise to new topological invariants. For example, in one dimension (1D), as $k$ is varied form 0 to $2\pi$, the eigenenergy trajectories $\{E_j(k)\}$ may form a “braid” (see Fig. 1 below). Two topologically distinct NH band structures (two braids) cannot be continuously deformed into each other while keeping the bands separable. Based on homotopy analysis, recent work established that the distinct topological sectors of 1D NH Hamiltonians with $N$ separable bands correspond to the conjugacy classes of the braid group $B_N$ [70, 71]. Unfortunately, homotopy theory alone does not offer an algorithm to compute the invariants directly from the Hamiltonian [72]. This raises the following open questions. (i) Given a generic NH Hamiltonian, how to determine its topological invariant? (ii) How to describe the phase transition between two topologically distinct phases? (iii) How to design a NH Hamiltonian whose bands form a desired braid pattern?

In this paper, we answer these questions by developing a knot theory for NH Hamiltonians. We prove that the topology of 1D NH Hamiltonians with separable bands is fully characterized by the knots (or links) formed by the eigenenergy strings, and the topological invariants are thus knot invariants. This is in sharp contrast to the various knots formed by zero-energy nodal lines in the 3D $k$-space of topological semimetals [73–81]. This perspective makes it straightforward to determine the phases, and predicts two types of phase transitions...
through EPs and accompanied by abrupt changes in the biorthogonal Wannier centers. We also present an algorithm to design tight-binding Hamiltonians to realize arbitrary knots, and demonstrate how the knot could be revealed from quantum quench.

**Knot classification of non-Hermitian band structures.** Our first main result is that 1D NH Hamiltonians with separable bands and no symmetry are completely classified by knots inside a solid torus. It follows that a topological invariant of the band structure must be a knot invariant. To prove this statement, first we summarize the results of Refs. [70, 71]. A 1D NH band structure with N separable bands defines a map from the Brillouin zone, a circle $S^1$, to the configuration space $X_N = (\text{Conf}_N \times F_N)/S_N$. Here $\text{Conf}_N$ is the ordered N-tuples of complex energy eigenvalues, the quotient space $F_N = U(N)/U^N(1)$ describes the energy eigenvectors, and $S_N$ is the permutation group. Since $\pi_1(F_N) = 0$, the equivalent classes of non-based map $[S^1, X_N]$ can be reduced to $[S^1, \text{Conf}_N/S_N]$, and further to the conjugacy classes of the braid group $B_N = \pi_1(\text{Conf}_N/S_N)$ [70, 71]. While this formal result based on homotopy theory is rigorous, the conjugacy classes of $B_N$ are hard to compute or visualize [82]. Here, we further relate them to knots. Notice that the braids of energy eigenvalues (constructed explicitly below) are closed due to the periodicity of the Brillouin zone, so the braid space is a solid torus. A theorem in knot theory dictates that two closed N-braids in $B_N$ can be smoothly deformed into each other in the solid torus iff they are conjugate to each other [82]. Thus, thanks to the one-to-one correspondence between the conjugacy class of N-braids and knots, we reach the conclusion that *knots provide a natural language to classify 1D NH Bloch bands.*

It is physically intuitive to construct the knot for a given 1D NH Hamiltonian $H(k)$. The procedure is outlined as follows. The complex eigenenergies form a set $\mathcal{E} = \{E_j(k)\}$ with band index $j = 1, ..., N$. They are the roots of the characteristic polynomial (ChP)

$$f(\lambda, k) = \det(\lambda - H(k)) = \prod_{j=1}^{N} (\lambda - E_j(k)). \quad (1)$$

As $k$ evolves from 0 to $2\pi$, the trajectory of $E_j(k)$ defines a *string* in the 3D space spanned by $(\text{Re}E, \text{Im}E, k)$. Overall N such strings may tangle with each to form a braid shown in Fig. 1. A braid can be faithfully described by its braid diagram obtained by projecting the N strings onto a chosen 2D plane parallel to the vertical $k$-axis. A braid diagram consists of a sequence of string crossings [83], each characterized by a *braid operator* $\tau_i$ in Artin’s notation. For instance, when projected on plane $\text{Im}E = +\infty$, $\tau_i (\tau_i^{-1})$ is defined by $\text{Re}E_i = \text{Re}E_{i+1}$ and $\text{Im}E_i < \text{Im}E_{i+1}$ ($\text{Im}E_i > \text{Im}E_{i+1}$). In other words, $\tau_i (\tau_i^{-1})$ indicates that the $i$-th string crosses over (under) the $(i+1)$-th string from left. Note that two non-adjacent braid operators commute: $\tau_i \tau_j = \tau_j \tau_i$ for $|j - i| \geq 2$, and $\tau_i \tau_{i+1} \tau_i = \tau_{i+1} \tau_i \tau_{i+1}$. The entire braid is then specified by its *braid word*, a product of braid operators, see Fig. 1. The set $\mathcal{E}$ is identical for $k = 0$ and $k = 2\pi$, so the braid is closed and becomes a knot (oriented with increasing $k$) in the $(\text{Re}E, \text{Im}E, k)$ space, which is topologically a solid torus. The end result of k evolution over one period $2\pi$ is the permutation

$$\sigma = \left( \begin{array}{cccc} E_1(0) & E_2(0) & \cdots & E_N(0) \\ E_1(2\pi) & E_2(2\pi) & \cdots & E_N(2\pi) \end{array} \right). \quad (2)$$

As usual, we define its parity $P(\sigma) = \pm 1$ if $\sigma$ can be expressed as even/odd number of transpositions.

The braid diagram may not be unique for a given band structure. Different choices of the projection plane yield isotopic braids related by Reidemeister moves, while different starting points of the k interval $[k_0, k_0 + 2\pi]$ correspond to braids within the same conjugacy class (this provides an understanding of why the conjugacy classes, not the elements, of $B_N$ are used for classification). These different choices however always yield the same unique knot, which is invariant under Reidemeister moves or translations along the torus axis. Thus using knots to describe the NH band structure is not only intuitively natural but also economical, free from the arbitrariness in representations. The knot structure of eigenenergy strings fully characterizes the topology of 1D NH Hamiltonians. And topologically distinct NH band structures correspond to distinct knots. Fig. 1 lists four braids and their associated knots, known as the Hopf link, trefoil knot, figure-8 knot, and Whitehead link, respectively. (To avoid clutter, hereafter we will refer to links also as knots.)

**Knot invariants.** It follows immediately that 1D NH bands are characterized by knot invariants [84]. This is in sharp contrast to the $\mathbb{Z}$ or $\mathbb{Z}_2$ invariants of Hermitian bands. A well-known invariant to discern inequivalent oriented knots is the Jones polynomial [85] $V_K(q)$, which can be calculated from the skein relation [82, 84],

$$q^{-1}V_{K_+} - qV_{K_-} + (q^{-1/2} - q^{1/2})V_{K_0} = 0. \quad (3)$$

Here $K_+, K_-, K_0$ refer to three oriented knots which only differ in a small region containing a string crossing as shown in Fig. 2(a). Starting from the Jones polynomial for trivial bands (i.e. an unlink of N strings) $V_O(q) = (-q^{-1/2} - q^{1/2})^{N-1}$, one can iteratively obtain the Jones polynomials for all other separable NH bands by the skein relation, through a series of string crossings [86].

Next we introduce a $\mathbb{Z}_2$ topological invariant $Q$ and relate it to the parity of band permutations defined earlier. For NH Hamiltonians, the right and left eigenvectors are defined as $H(k)|\psi_n\rangle = E_n(k)|\psi_n\rangle$ and $H^\dagger(k)|\chi_n\rangle = E_n^*(k)|\chi_n\rangle$, which satisfy the biorthogonal normalization $\langle \chi_m|\psi_n\rangle = \delta_{mn}$ [87]. Define the non-Abelian Berry connection $A_{B}^{mn} = i(\langle \chi_m|\partial_k|\psi_n\rangle$ and the global biorthogonal
Berry phase [88]

\[ Q = \oint_{C} e^{2\pi i} \text{Tr}[A_B]. \]  

One can prove [89] that \( Q \) is quantized to 0 (\( \pi \)) when the band permutation \( \sigma \) is even (odd),

\[ e^{iQ} = (-1)^{P(\sigma)}. \]  

While \( Q \) is indeed a knot invariant, due to its \( \mathbb{Z}_2 \) nature it only coarsely classifies knots into two groups. For example, the Hopf and figure-8 knot have the same \( Q = 0 \), and similarly trefoil and Whitehead knot have \( Q = \pi \).

In Hermitian systems, Wilson loop provides a powerful characterization of band topology [90–92]. For NH systems, we define the biorthogonal Wilson loop from the Berry connection

\[ W_B = \mathcal{P} e^{i \frac{2\pi}{\sqrt{N}} \int dk} A_B, \]  

where \( \mathcal{P} \) denotes path ordering. Its eigenphases \( \nu_n \), defined by \( W_B|\mu_n\rangle = e^{i\nu_n}|\mu_n\rangle \), are the Wannier centers [28, 93, 94]. It can be shown [89] that \( Q = \sum_n \nu_n \).

A toy model: the twistor Hamiltonian. To illustrate different knots and their phase transitions, we introduce a simple two-band NH Hamiltonian

\[ T_n = \begin{pmatrix} 0 & e^{i\alpha_n} \\ 1 & 0 \end{pmatrix}, \]  

where \( n \) counts the number of twists of the two band strings, \( E_{\pm} = \pm e^{i\alpha_n} \), as \( k \) evolves from 0 to \( 2\pi \). The braid word of \( T_n \) is simply \( \tau_n^0 \). The twistor Hamiltonian \( T_n \) for \( n = 0, 1, 2 \) gives rise to the unlink, unknot, and Hopf link, respectively. We will use \( T_n \) as building block to construct a model with two tunable parameters \( (m_1, m_2) \),

\[ H_{12}(k) = im_1\tau_1 + m_2 T_1 + T_2. \]  

It has three topologically distinct phases, the Hopf link (blue region), the unlink (green), and the unknot (pink) phase, see the phase diagram in Fig. 2(b). The phase boundaries are given by \( m_1^2 + m_2^2 = 1 \) and \( m_2 = \pm m_1 - 1 \). The knot topology is apparent from the two eigenenergy strings (blue and red solid lines in insets). For the unlink, the two strings do not braid, each forming a loop; for the Hopf link, the two strings braid twice, and the two loops are linked; for the unknot, the two strings braid once to form one single loop. We emphasize that all three phases here exhibit NH skin effect [40–54] because projecting the knot onto the complex \( E \) plane yields a band structure (dash lines) with a point gap [65–67]. Previous classification framework [55–60] based on line/point gaps however cannot distinguish these phases or describe their phase transitions. The classification presented here based on knots is finer and complete.

Phase transition through exceptional points. A transition between two phases characterized by different knots must occur through the crossing of the strings, i.e., through band degeneracy points. There are two kinds of band degeneracies in NH systems, the exceptional point (EP) or non-defective degeneracy point (NDP). The key difference is that EPs are defective, where the eigenvectors coalesce, leaving the Hamiltonian non-diagonalizable, while at an NDP, the eigenstates remain distinct. For a general 1D NH band with no symmetry, NDPs are unstable and will split into several EPs by small perturbations [95]. Thus we are led to the conclusion that a quantum phase transition between phases of distinct knots is accompanied by exceptional points.

There are two scenarios for two strings to undergo a “knot transition” as sketched in Fig. 2(a). In a type-I transition, the braid word \( \tau_i^{\pm t} \rightarrow \tau_i^0 \), i.e., the two strings change from cross to no-cross (or vice versa) by going through an EP, and \( Q \) changes. One example is trefoil knot transforming to Hopf link via \( \tau_1 \rightarrow \tau_1^0 \). A type-II transition occurs when the braid word \( \tau_i \rightarrow \tau_i^{-1} \), i.e., an over-cross becomes an under-cross or vice versa. It is usually accompanied by two EPs, and \( Q \) remains the same. Most generally, any two phases can be connected through a series of transitions of either type. For \( H_{12}(k) \), the transition from the Hopf link to the unknot along the line \( m_1 = m_2 \) belongs to type I and the EP is located at \( (m_1, k) = (1/\sqrt{2}, \pi) \), as shown in Fig. 2(c). The transi-
tion from the Hopf link to the unlink along the $m_2 = 0$ line is of type II, with two EPs located at $(m_1, k) = (1, 0)$ and $(1, \pi)$ as shown in Fig. 2(d). Note that the Wannier centers undergo abrupt changes at these transitions, see Fig. 2(d) and (f).

**How to design knotty Hamiltonians.** Beyond these simple knots, it becomes challenging to construct the tight-binding Hamiltonian $H_K(k)$ whose bands tie into certain given knot $K$. Here we outline a solution to this problem, which aids the experimental realization and probe of NH knots. The key is to find a CHP $f(\lambda, k)$ with $\lambda \in \mathbb{C}$ and $k \in [0, 2\pi]$ whose roots produce the desired eigenenergy strings. Our algorithm consists of two steps [89].

In the first step, $f(\lambda, k)$ is constructed from the data of $K$. From the braid diagram of $K$, decompose the permutation $\sigma$ into a series of cycles $\sigma = s_1 s_2 \ldots$ with $l_n$ the length of cycle $s_n$. For each cycle, standard trigonometrical parametrization [89, 96] generates two real functions $F_n(k), G_n(k)$. The strings in cycle $s_n$ are given by coordinates $(F_n(k_{n1}), G_n(k_{n1})), k_{n1} = (k + 2\pi j_n)/l_n$ and $j_n = 0, \ldots, l_n - 1$. Thus the roots of the following CHP

$$f(\lambda, k) = \prod_{n, j_n}(\lambda - F_n(k_{n1}) - i G_n(k_{n1}^\prime))$$

yield the desired knot $K$. The CHP obtained is a power series of $\lambda$, $f(\lambda, k) = \lambda^N + \sum_{j=0}^{N-1} \zeta_j(k)\lambda^j$, where $\zeta_j(k)$ is a Laurent series of $e^{\pm ik}$. In the second step, Hamiltonian $H_K$ is constructed from $f(\lambda, k)$ above: it is a sparse matrix [89] with the only non-zero elements being

$$H_K^{i,j} = 1, \quad i = 1, 2, \ldots, N - 1;$$

$$H_K^{i,1} = -\zeta_{N-i}(k), \quad i = 1, 2, \ldots, N. \quad (10)$$

For example, applying this algorithm to braid word $\tau_1^3$ reproduces the twistor Hamiltonian $T_{13}$. The NH Hamiltonians for the figure-8 knot and Whitehead link, $H_8$ and $H_w$ shown in Fig. 1, are similarly obtained. Their explicit expressions are lengthy and can be found in [89]. More tangled knots require longer-range couplings.

**Revealing knots from quantum quench.** A direct probe of the knots would require exhaustive measurements of $\{E_j(k)\}$, e.g. by tracing the oscillation and growth/decay in dynamics, which seems daunting. An alternative is to probe the eigenstates. As an example, consider the two-band system $H_{12}(k)$ where the eigenstates can be accessed via Bloch state tomography [97-101]. Each of the two right eigenstates $|\psi_{1,2}(k)\rangle$ corresponds to a point on the Bloch sphere. As $k$ is varied, their trajectories trace out two curves (in red and blue) on the Bloch sphere as illustrated in Fig. 3. For the Hopf-link phase (a), each curve is a closed loop, and they intersect twice. In the unlink phase (c), we have two closed loops but they remain separated. Note that both phases have even permutation parity, $Q = 0$. In contrast, in the unknot phase (b), the red curve joins the blue curve to form a single loop, and $Q = \pi$. It is clear from this example that different knots may be distinguished from Bloch state tomography, and the invariant $Q$ can be read out directly.

![FIG. 3. Signatures of knots after quantum quench. The red/blue curves are the eigenvectors $|\psi_{1,2}(k)\rangle$ of $H_{12}(k)$ on the Bloch sphere. From an initial state $|\xi_0\rangle = (1, 0)^T$ (north pole), the state evolves with $H_{12}(k)$ and after a long time falls into the solid line part of the eigenstates. The arrow denotes increasing $k$ from 0 to $2\pi$, and the purple (green) dots represent the $k = 0$ ($k = \pi$) mode. The parameters are (a) $m_1 = m_2 = 0.5$, the Hopf-link phase; (b) $m_1 = m_2 = 0.9$, the unknot phase; and (c) $m_1 = 1.2, m_2 = 0$, the unlink phase.](image-url)
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Supplementary Materials

In this Supplementary material, we provide details on (I) the proof of relations between the global biorthogonal Berry phase $Q$, band permutation $\sigma$ and Wilson loop $W_B$; (II) the algorithm of constructing a tight-binding Hamiltonian $H_K(k)$ associated with a given knot $K$ and explicit examples of figure-8 knot and Whitehead link.

I. Relation between biorthogonal Berry phase, band permutation and Wilson loop

For a non-Hermitian (NH) Hamiltonian $H(k)$, its right and left eigenvectors are defined as

$$H(k)|\psi_n\rangle = E_n(k)|\psi_n\rangle, \quad H^\dagger(k)|\chi_n\rangle = E_n^*(k)|\chi_n\rangle.$$  \hfill (11)

The two types of eigenvectors satisfy the biorthogonal normalization $\langle \gamma_n | \psi_n \rangle = \delta_{mn}$. The global biorthogonal Berry phase is defined as $Q = \oint_0^{2\pi} dk \; \text{Tr}[A_B]$. Here $A_B$ is the non-Abelian Berry connection matrix, with its $(m,n)$-element $A_{Bmn} = i\langle \chi_m | \partial_k | \psi_n \rangle$. First, $Q$ is only well-defined modulo $2\pi$. In fact, a gauge transformation (note the biorthogonal normalization should be imposed)

$$|\psi_n\rangle \rightarrow e^{-i\phi(k)}|\psi_n\rangle, \quad |\chi_n\rangle \rightarrow e^{i\phi(k)}|\chi_n\rangle$$  \hfill (12)

brings $A_B$ to $\tilde{A}_B = A_B + \partial_k \phi(k)$. $\phi(k)$ is a continuous single-valued function on $k \in [0, 2\pi]$ satisfying $\phi(k = 0) = \phi(k = 2\pi)$. The gauge transformation takes $Q$ to $\tilde{Q} = Q + 2\pi p$ ($p \in \mathbb{Z}$). Using all the $N$ right eigenstates, we define an $N \times N$ matrix $\Psi = (|\psi_1\rangle, |\psi_2\rangle, ..., |\psi_N\rangle)$. The global biorthogonal Berry phase is recast into

$$Q = i \oint_0^{2\pi} dk \; \text{Tr}[\Psi^{-1} \partial_k \Psi] = i \oint_0^{2\pi} dk \; \partial_k \text{Tr}[\log \Psi] = i \log \frac{\det[\Psi(k = 2\pi)]}{\det[\Psi(k = 0)]}. \hfill (13)$$

The periodicity of Hamiltonian $H(k) = H(k + 2\pi)$ dictates that the whole eigenvector set to be identical at $k = 0$ and $k = 2\pi$. However due to band braiding, each eigenvector $|\psi_j\rangle$ does not necessarily return to itself by evolving from $k = 0$ to $k = 2\pi$. The braiding is labeled by the band permutation $\sigma$ (see Eq. (2) in the main text). It is clear from Eq. (13) that if the permutation is even, $\det \Psi(k = 2\pi) = \det \Psi(k = 0)$, $Q = 0$; if the permutation is odd, $\det \Psi(k = 2\pi) = -\det \Psi(k = 0)$, $Q = \pi$. Hence $Q$ relates to the parity of band permutations through

$$(-1)^{P(\sigma)} = e^{i\pi Q}. \hfill (14)$$

Next we turn to the biorthogonal Wilson loop $W_B$ (see its definition in Eq. (6) in the main text). In discretized form, $W_B$ is expanded as

$$W_B = \lim_{M \rightarrow \infty} W_b(k_{M-1})W_b(k_{M-2})...W_b(k_1)W_b(k_0). \hfill (15)$$

Here $k_j = \frac{2\pi j}{N}$, $\Delta k = \frac{2\pi}{N}$, and $W_{Bmn}(k_j) = \langle \chi_m(k_j + \Delta k) | \psi_n(k_j) \rangle$. By diagonalizing $W_B$, i.e., $W_B|\mu_n\rangle = e^{i\nu_n}|\mu_n\rangle$, we get $N$ Wannier centers $\nu_n$ ($1 \leq n \leq N$). The total Wannier center can be calculated as

$$\lim_{M \rightarrow \infty} \sum_{n=1}^N \nu_n = \lim_{M \rightarrow \infty} -i \text{Tr} \log[W_B]$$

$$= \lim_{M \rightarrow \infty} -i \log \text{det}[W_B]$$

$$= \lim_{M \rightarrow \infty} -i \sum_{j=0}^{M-1} \log \text{det}[W_b(k_j)]$$

$$= \lim_{M \rightarrow \infty} -i \sum_{j=0}^{M-1} \sum_{n=1}^N \log[(\chi_n(k_j + \Delta k)|\psi_n(k_j)\rangle]$$

$$= \oint_0^{2\pi} dk \; \text{Tr}[A_B] = Q. \hfill (16)$$

We check the above relations using the twistor model $T_n$ (see Eq. (7) in the main text). The two eigenbands of $T_n$ and $T_n^\dagger$ are $E_{\pm} = \pm e^{\frac{\pi i n}{2}}$ and $E_{\pm}^* = \pm e^{-\frac{\pi i n}{2}}$, with their corresponding right and left eigenvectors:

$$|\psi_\pm\rangle = \frac{1}{\sqrt{2}} \left( e^{\frac{\pi i n}{2}} \pm 1 \right); \quad |\chi_\pm\rangle = \frac{1}{\sqrt{2}} \left( e^{\frac{\pi i n}{2}} \pm 1 \right). \hfill (17)$$
Obviously $|\psi_{\pm}\rangle$ and $|\chi_{\pm}\rangle$ satisfy the biorthogonal normalization relation. The Berry connection is

$$i \langle \chi_{\pm} | \partial_k | \psi_{\pm} \rangle = -\frac{n}{4},$$  \hspace{1cm} (18)$$
yielding $Q = -n\pi$. The Wannier centers are $\nu_+ = \pi n$, $\nu_- = 0$. For Hamiltonian $T_n$, $n$ labels the braiding times of the two eigenbands $E_{\pm}$ by evolving $k$ from 0 to $2n$. The simplest cases of $n = 0, 1, 2, 3$ correspond to unlink, unknot, Hopf link, and trefoil knot, respectively. If $n$ is even, the two bands exchange even times and the permutation $\sigma$ is even; If $n$ is odd, the two bands exchange odd times and the permutation $\sigma$ is odd. Eq. (14) is verified.

II. Construction of tight-binding Hamiltonian $H_K(k)$ associated with a given knot $K$

In the main text, we have outlined the algorithm to generate a NH Hamiltonian $H_K(k)$ corresponding to an arbitrary knot $K$. The algorithm is decomposed into two steps. The first step is to find a characteristic polynomial (ChP) $f(\lambda, k)$ ($\lambda \in \mathbb{C}, k \in [0, 2\pi]$) such that its roots form the desired knot $K$. Note that $f(\lambda, k)$ is a complex-valued polynomial and contains three real variables $\text{Re}\lambda$, $\text{Im}\lambda$, $k$. Hence its roots can be regarded as the intersection of the two surface determined by $\text{Re}f = 0$ and $\text{Im}f = 0$. The second step is to construct the tight-binding Hamiltonian $H_K(k)$ with $f(\lambda, k)$ as its ChP. In our algorithm, the ChP is a power series of $\lambda$ and Laurent series of $e^{\pm ik}$. Here we detail the above steps and showcase the procedures with the figure-8 knot and Whitehead link.

**Step-1** In the first step, we need to parameterize the knot $K$, which is presented by a braid diagram $B_K$ [96]. Note that while $B_K$ is not unique, different choices of $B_K$ either correspond to braids related by Reidemeister moves or braids inside the same conjugacy class. We choose one specific diagram and plot it on the $xz$ plane (see Fig. 1 in the main text). The vertical $z$-axis denotes $k$ direction. For simplicity, the diagram $B_K$ is plotted in a way where the crossings are evenly distributed along the $z$-axis. Suppose there are $c[K]$ crossings in total. They are located at

$$k_m = \frac{\pi}{c[K]} (2m - 1), \quad m = 1, 2, ..., c[K].$$  \hspace{1cm} (19)$$
In the two-dimensional (2D) braid-diagram presentation, each strand of $B_K$ is a piecewise linear function of $k$. $B_K$ represents for $N$ strings in 3D, with trajectories $(F_j(k), G_j(k), k)$, $j = 1, 2, ..., N$. Here $F_j(k)$ and $G_j(k)$ are real functions of $k$. Our task is to obtain $F_j(k)$ and $G_j(k)$ from $B_K$. Due to string braiding, $F_j(k)$ and $G_j(k)$ are in general not $2\pi$-periodic. However $F_j(2\pi) = F_j(0)$ and $G_j(2\pi) = G_j(0)$ always hold for some $1 \leq j' \leq N$ ($k = 0$ and $k = 2\pi$ are identical). This motivates us to obtain $F_j(k)$ (same for $G_j(k)$) from a parent function, where each $F_j(k)$ corresponds to a piece of the parent function.

The $N$ strings are associated with an element $\sigma$ of the permutation group $S_N$, as defined in Eq. (2) in the main text. In group theory, $\sigma$ can be decomposed into a sequence of cycles $\sigma = s_1 s_2 ...$. We denote $\mathcal{C}_K = \{ s_1, s_2, ... \}$ as the set of cycles, which gives all the link components of the closure of $B_K$ (or knot $K$). For a given cycle $s_n \in \mathcal{C}_K$, we denote $l_n$ as its length. Inside each cycle $s_n$, we rearrange its $l_n$ string indices to be from 0 to $l_n - 1$ such that the end point of $j_n$-th string at $k = 2\pi$ is the starting point of the $(j_n + 1)$-th string at $k = 0$ for every $0 \leq j_n \leq l_n - 1$. Using the above notations, any string of the diagram $B_K$ is specified by a pair of indices $(s_n, j_n)$, with $s_n \in \mathcal{C}_K$, $j_n = 0, 1, ..., l_n - 1$. We assign two continuous real functions $F_n(k)$ and $G_n(k)$ as parent functions, which are $2\pi$-periodic, for each link component $s_n$. The $j_n$-th string inside $s_n$ takes

$$F_{j_n}(k) = F_n(k^j_n), \quad G_{j_n}(k) = G_n(k^j_n), \quad \text{with} \quad j_n = 0, 1, ..., l_n - 1, \quad k \in [0, 2\pi],$$  \hspace{1cm} (20)$$
where $k^j_n = (k + 2\pi j_n)/l_n$. Next we demonstrate how to obtain $F_n(k)$ and $G_n(k)$ of each cycle $s_n$ from the trigonometric interpolation of the diagram $B_K$. To get $F_n(k)$, we first neglect the crossings of $B_K$ while encode the crossing information into $G_n(k)$. For cycle $s_n$, we define a piecewise linear function $L_n(k)$ on $k \in [0, 2\pi]$:

$$L_n(k^j_n) = B_K(k)_{s_n, j_n}, \quad \text{with} \quad j_n = 0, 1, ..., l_n - 1; \quad s_n \in \mathcal{C}_K.$$  \hspace{1cm} (21)$$
Here $B_K(k)_{s_n, j_n}$ denotes the $(s_n, j_n)$-th string of $B_K(k)$. The trigonometric interpolation of $F_n(k)$ is through the following $c[K] l_n$ points located at

$$\left( \frac{k^m}{l_n} - \frac{\pi}{c[K] l_n}, L_n \left( \frac{k^m}{l_n} - \frac{\pi}{c[K] l_n} \right) \right), \quad m = 1, 2, ..., c[K] l_n.$$  \hspace{1cm} (22)$$
The interpolation data is evenly distributed along \( k \) direction, hence the interpolation is the Fourier transformation:

\[
F_n(k) = \sum_{m=-c[K]|n|/2+1}^{c[K]|n|/2} a_m e^{imk} + a_{c[K]|n|/2} \cos \left( \frac{c[K]|n|}{2} k \right), \quad \text{if } c[K]|n| = \text{even},
\]

\[
F_n(k) = \sum_{m=-c[K]|n|/2+1/2}^{c[K]|n|/2-1/2} a_m e^{imk}, \quad \text{if } c[K]|n| = \text{odd},
\]

where the Fourier coefficients are

\[
a_m = \frac{1}{c[K]|n|} \sum_{n=0}^{c[K]|n|-1} L_n \left( \frac{k_n}{l_n} - \frac{\pi}{c[K]|n|} \right) e^{-i \left( \frac{k_n}{l_n} - \frac{\pi}{c[K]|n|} \right) m}.
\]

Having obtained \( F_n(k) \) for all cycles \( s_n \in \mathcal{C}_K \), the next step is to determine \( G_n(k) \) from \( F_n(k) \) by incorporating the string crossings. Each crossing is assigned a \( + \) or \( - \) sign from the braid diagram \( B_K \). We denote the \( z \)-coordinate of the crossing point as \( k_p \), which are the solutions of

\[
F_n(\frac{k_p + 2\pi j_n}{l_n}) = F_n(\frac{k_p + 2\pi j_n'}{l_n' }), \quad \text{for all } s_n, s_n' \in \mathcal{C}_K; \ j_n = 0, 1, ..., l_n - 1; \ j_n' = 0, 1, ..., l_n' - 1.
\]

The interpolation data for \( G_n(k) \) is chosen as \( \frac{k_p + 2\pi j_n}{l_n}, \text{sgn}(k_p) \). Here \( \text{sgn}(k_p) = \pm 1 \) if the crossing at \( k_p \) is an under/over crossings in the diagram \( B_K \). Compared to \( F_n(k) \), usually the interpolation data of \( G_n(k) \) is not evenly distributed along \( k \) direction. Suppose there are \( c[F_n] \) crossing points (including both crossings with itself and other component \( n' \in \mathcal{C}_K \)). Formally, we set the interpolation function as

\[
G_n(k) = \sum_{m=-c[F_n]/2+1}^{c[F_n]/2} b_m e^{imk} + b_{c[F_n]}/2 \cos \left( \frac{c[F_n]}{2} k \right), \quad \text{if } c[F_n] = \text{even},
\]

\[
G_n(k) = \sum_{m=-c[F_n]/2+1/2}^{c[F_n]/2-1/2} b_m e^{imk}, \quad \text{if } c[F_n] = \text{odd},
\]

The interpolation coefficient \( b_m \) can be obtained by solving a matrix equation using the above interpolation data.

Through the above procedures, the strings of knot \( K \) are parameterized by \( (F_n(k^n_j), G_n(k^n_j), k) \), with \( s_n \in \mathcal{C}_K \), \( j_n = 0, 1, ..., l_n - 1 \). The desired ChP with such \( N \) strings as its roots are

\[
f(\lambda, k) = \prod_{s_n \in \mathcal{C}_K} \prod_{j_n = 0}^{l_n-1} [\lambda - F_n(k^n_j) - iG_n(k^n_j)].
\]

Step-2 The second step is to generate an \( N \) by \( N \) NH Hamiltonian \( H_K(k) \), with \( f(\lambda, k) \) as its ChP. To this end, we expand \( f(\lambda, k) \) in the powers of \( \lambda \),

\[
f(\lambda, k) = \lambda^N + \sum_{j=0}^{N-1} \zeta_j(k) \lambda^j,
\]

where \( \zeta_j(k) (j = 0, 1, ..., N - 1) \) is a Laurent series of \( e^{\pm ik} \). There are many different choices of \( H_K(k) \), corresponding to the same ChP. In the main text, we have set \( H_K(k) \) as the following simple form:

\[
H_K(k) = \begin{pmatrix}
-\zeta_{N-1}(k) & -\zeta_{N-2}(k) & \cdots & -\zeta_1(k) & -\zeta_0(k) \\
1 & 0 & 0 & \cdots & 0 \\
0 & 1 & 0 & 0 & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
0 & 1 & 0 & 0 & \cdots \\
\end{pmatrix}.
\]

It is easy to check \( \det(\lambda - H_K(k)) = f(\lambda, k) \).
We showcase the above procedures by explicitly working out the figure-8 knot. The similar, we can work out the NH Hamiltonian \( H_{K}(k) \) for the Whitehead link. The braid diagram \( B_{K} \) (see Fig. 1 in the main text) is described by braid word \( \tau_{1} \tau_{2}^{-1} \tau_{1} \tau_{2}^{-1} \tau_{1} \), with total crossing number \( c[K] = 5 \). The permutation associated with \( B_{K} \) is \( \sigma = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \). There are two cycles \( \sigma = (13)(2) \) in \( \sigma \). \( s_{1} = (13) \) with length \( l_{1} = 2 \) and \( s_{2} = (2) \) with length \( l_{2} = 1 \).
To parameterize the two cycles, we need to identify all the data points of trigonometric interpolation. For cycle $s_1$, we pick $c[K]_1 = 10$ evenly distributed points along $k$ direction, with coordinates $(0, -1), (\frac{\pi}{5}, 0), (\frac{2\pi}{5}, 1), (\frac{3\pi}{5}, 1), (\frac{4\pi}{5}, 0), (\pi, 1), (\frac{6\pi}{5}, 1), (\frac{7\pi}{5}, 0), (\frac{8\pi}{5}, -1), (\frac{9\pi}{5}, -1)$ on the $xz$ plane. For cycle $s_2$, we pick $c[K]_2 = 5$ evenly distributed points with coordinates $(0, 0), (\frac{\pi}{2}, -1), (\frac{3\pi}{2}, -1), (\frac{5\pi}{2}, 0), (\frac{7\pi}{2}, 1)$. The discrete Fourier transformation yields

$$F_1(k) = 0.1 - 0.79 \cos k + 0.57 \sin k - 0.16 \cos 2k + 0.5 \sin 2k - 0.11 \cos 3k - 0.35 \sin 3k$$
$$+ 0.06 \cos 4k + 0.04 \sin 4k - 0.1 \cos 5k,$$
$$F_2(k) = -0.2 + 0.32 \cos k - \sin k - 0.12 \cos 2k - 0.09 \sin 2k. \tag{34}$$

To obtain $G_1(k)$ and $G_2(k)$, we solve all the crossings of the three strings $F_1(\frac{k}{2}), F_1(\frac{k+2\pi}{2})$, and $F_2(k)$ inside $[0, 2\pi]$. The solution of $F_1(\frac{k}{2}) = F_1(\frac{k+2\pi}{2})$ is $k_p = 1.8850$: The solutions of $F_1(\frac{k}{2}) = F_2(k)$ are $k_{p_1} = 0.6004, 4.2329, 5.8202$: The solution of $F_1(\frac{k+2\pi}{2}) = F_2(k)$ is $k_p = 3.1696$. The interpolation data for $G_1(k)$ and $G_2(k)$ on the $yz$ plane are respectively $(\frac{0.6004}{2}, -1), (\frac{1.8850}{2}, 1), (\frac{4.2329}{2}, -1), (\frac{5.8208}{2}, 1), (\frac{1.8850+2\pi}{2}, -1), (\frac{3.1696+2\pi}{2}, 1)$ and $(0.6004, 1), (3.1695, -1), (4.2329, 1), (5.8202, -1)$. The trigonometric interpolation reads

$$G_1(k) = 0.26 + 0.11 \cos k - 0.40 \sin k - 0.27 \cos 2k - 0.37 \sin 2k - 1.32 \cos 3k,$$
$$G_2(k) = 1.03 - 0.12 \cos k + 1.47 \sin k - 2.11 \cos 2k. \tag{35}$$

According to Eq. (27), the ChP is

$$f(\lambda, k) = [\lambda - F_2(k) - iG_2(k)] \prod_{j=0}^{1}[\lambda - F_1(\frac{k+2\pi j}{2}) - iG_1(\frac{k+2\pi j}{2})]$$

$$= \lambda^3 + \zeta_2(k)\lambda^2 + \zeta_1(k)\lambda + \zeta_0(k). \tag{36}$$

where

$$\zeta_2(k) = -1.56i + 0.66i \cos k - 0.74i \sin k + 2.11 \cos 2k,$$
$$\zeta_1(k) = (-0.25 + 1.07i) - (0.01 + 1.22i) \cos k + (0.34 + 1.04i) \sin k + (0.36 - 2.14i) \cos 2k + (0.73 + 0.64i) \sin 2k$$
$$+ (0.37 + 0.13i) \cos 3k - (0.83 + 1.44i) \sin 3k - (0.01 + 0.26i) \cos 4k - (0.04 + 0.09i) \sin 4k,$$
$$\zeta_0(k) = (0.19 - 1.05i) + (0.77 + 0.76i) \cos k - (0.07 + 0.54i) \sin k - (0.40 - 1.61i) \cos 2k - (0.64 - 0.23i) \sin 2k$$
$$+(1.26 - 1.28i) \cos 3k - (0.37 + 0.39i) \sin 3k + (0.73 - 0.33i) \cos 4k - (0.47 + 0.44i) \sin 4k$$
$$+(0.22 + 0.88i) \cos 5k + (0.51 - 0.06i) \sin 5k + (0.14 - 0.02i) \cos 6k - 0.04i \sin 6k - 0.01i \cos 7k. \tag{37}$$

The NH Hamiltonian $H_w(k)$ follows from Eq. (29) with $\zeta_j(k)$ ($j = 0, 1, 2$) listed above.