SUPPLEMENTARY MATERIAL FOR "KNOT TOPOLOGY IN QUANTUM SPIN SYSTEM"

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A: Bloch vector and winding number

The planar Bloch vector in the plane B_x-B_y for the situations shown in Fig. 1 of the main text is depicted in Fig. S1. The winding of Bloch vector around the origin (black dot) of B_x-B_y plane in the gapped phase is w. The arrows indicate the direction of the curves as k increasing from 0 to 2π; the counterclockwise (clockwise) direction yields the $+$ $(-)$ sign of the winding number. In the first and third rows, the curve of Bloch vector encloses the origin one to five times from the left to right, and the winding number in Eq. (6) of the main text is $w = \pm 1$ to $w = \pm 5$, respectively. In the second and fourth rows, the curve of Bloch vector passes through the origin. Thus, the winding number of the effective planar magnetic field is not well-defined in the gapless phase.

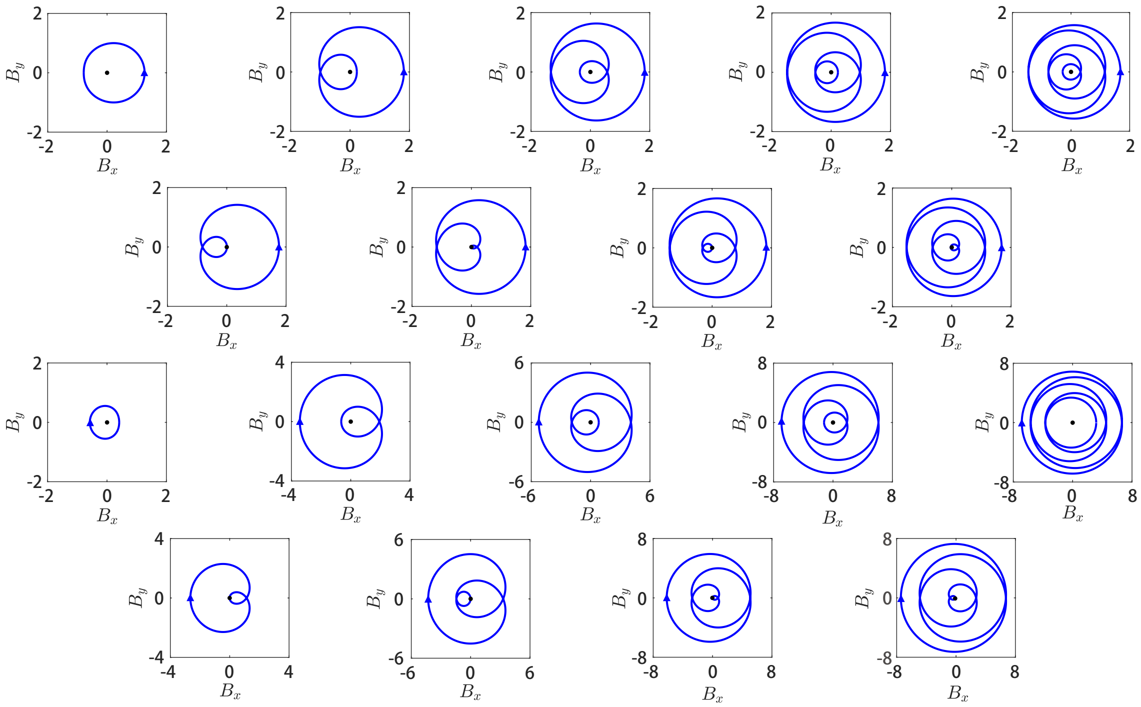

FIG. S1. Curve of Bloch vector in the B_x-B_y plane, the black dot is the origin. The corresponding knot or link eigenstate graph is depicted in Fig. 1 of the main text.

B: Linking number

In the gapped phase, the eigenstates $\left|\psi_k^{\pm}\right\rangle$ are represented by two loops on a torus surface, forming a torus link [Fig. S2(a)]. $\mathbf{r}_+(k)$ (blue loop) and $\mathbf{r}_-(k')$ (red loop) represent the positive branch $\left|\psi_k^{+}\right\rangle$ and the negative branch $\left|\psi_{k'}^{-}\right\rangle$, respectively. We construct a vector field

$$\mathbf{h}(k,k') = \mathbf{r}_+(k) - \mathbf{r}_-(k'), \tag{1}$$

where $\mathbf{r}_+(k)$ and $\mathbf{r}_-(k')$ in the cylindrical coordinate [Fig. S2(b)] are expressed as

$$\begin{aligned}\mathbf{r}_+(k) &= 0\hat{\boldsymbol{\theta}} + r\sin\varphi_+(k)\,\hat{\mathbf{z}} + [R + r\cos\varphi_+(k)]\,\hat{\mathbf{r}},\\ \mathbf{r}_-(k') &= 0\hat{\boldsymbol{\theta}}' + r\sin\varphi_-(k')\,\hat{\mathbf{z}}' + [R + r\cos\varphi_-(k')]\,\hat{\mathbf{r}}'.\end{aligned} \tag{2}$$

On the torus, R (in red) is the distance from the center of the tube to the center of the torus, and r (in purple) is the radius of the tube. Two cylindrical coordinates are related as follows

$$\hat{\mathbf{z}}' = \hat{\mathbf{z}}, \hat{\mathbf{r}}' = \cos(k'-k)\,\hat{\mathbf{r}} + \sin(k'-k)\,\hat{\boldsymbol{\theta}}. \tag{3}$$

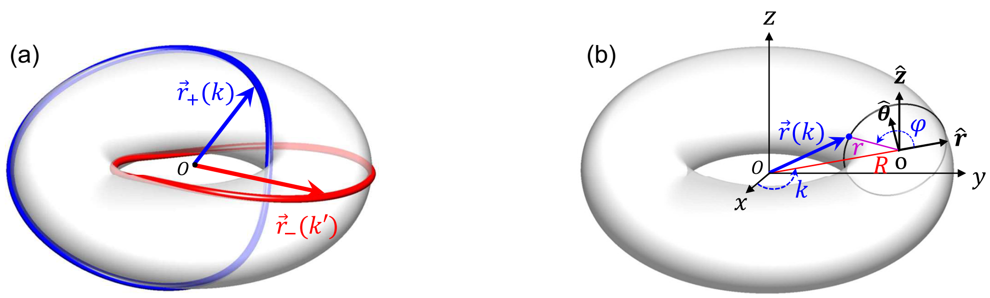

FIG. S2. (a) A two-component Hopf link lies on the torus surface, each component is a closed loop of the eigenstate $|\psi_k^\pm\rangle$. (b) The cylindrical coordinate for the torus.

Besides, we have $\varphi_-(k) = \varphi_+(k) + \pi$ and $\varphi_-(k') = \varphi_+(k') + \pi$. Based on these relations, we have

$$\mathbf{h}(k, k') = h_\theta \hat{\boldsymbol{\theta}} + h_z \hat{\mathbf{z}} + h_r \hat{\mathbf{r}}, \tag{4}$$

where

$$\begin{aligned} h_\theta &= [R - r\cos\varphi_+(k')]\sin(k - k'), \\ h_z &= r\sin\varphi_+(k) + r\sin\varphi_+(k'), \\ h_r &= R + r\cos\varphi_+(k) - [R - r\cos\varphi_+(k')]\cos(k - k'). \end{aligned} \tag{5}$$

Each point (k, k') is mapped to a three-dimensional vector $\mathbf{h}$. Since k and k' are periodic parameters, the endpoint of vector $\mathbf{h}$ draws a deformed torus surface in the $(\boldsymbol{\theta}, \mathbf{z}, \mathbf{r})$ space.

After introducing the vector field $\mathbf{h}$, we note that the linking number of two curves $\mathbf{r}_+(k)$ and $\mathbf{r}_-(k')$ in Eq. (8) of the main text can be expressed in the form of

$$L = \frac{1}{4\pi} \oint_k \oint_{k'} \frac{\mathbf{h}}{|\mathbf{h}|^3} \cdot \left(\frac{\partial \mathbf{h}}{\partial k} \mathrm{d}k \times \frac{\partial \mathbf{h}}{\partial k'} \mathrm{d}k'\right). \tag{6}$$

Mathematically, the above expression of linking number is equal to the solid angle subtended by the deformed torus surface divided by 4π [1]. Since the deformed torus is irregularly shaped and solid angle is hard to be calculated, we choose a cross section that contains the origin $(0, 0, 0)$ in the $(\boldsymbol{\theta}, \mathbf{z}, \mathbf{r})$ space, whose plane angle of the curve in the cross section of the deformed torus surface is half the solid angle. By doing this, we can easily get the solid angle of the deformed torus and then obtain corresponding linking number.

To get the cross section containing the origin, we set $h_\theta = 0$. The $h_\theta = 0$ plane cuts off the deformed torus surface to a curve in the $(\mathbf{z}, \mathbf{r})$ plane. By setting $h_\theta = 0$, we have $k' = k$ and $\mathbf{h}$ is reduced to

$$\mathbf{h} = h_z \hat{\mathbf{z}} + h_r \hat{\mathbf{r}} = 2r\sin\varphi_+(k)\,\hat{\mathbf{z}} + 2r\cos\varphi_+(k)\,\hat{\mathbf{r}}, \tag{7}$$

which indicates a closed circle Γ centered at $(0, 0)$ in the $(\mathbf{z}, \mathbf{r})$ plane and the linking number defined by the vector field $\mathbf{h}$ is given by

$$\begin{aligned} L &= \frac{1}{2\pi} \oint_\Gamma \frac{1}{4r^2} (h_z \nabla_k h_r - h_r \nabla_k h_z) \mathrm{d}k \\ &= -\frac{1}{2\pi} \int_0^{2\pi} \nabla_k \varphi_+(k)\, \mathrm{d}k. \end{aligned} \tag{8}$$

Furthermore, from the definition $\varphi_+(k) = \arctan(-B_y/B_x)$, the linking number Eq. (8) can be expressed as

$$L = \frac{1}{2\pi} \oint_C \frac{1}{B^2} (B_x \mathrm{d}B_y - B_y \mathrm{d}B_x) = w. \tag{9}$$

The linking number L is equivalent to the winding number w defined in Eq. (6) of the main text.

[1] J. K. Asbóth, L. Oroszlány, and A. Pályi, *A Short Course on Topological Insulators: Band-structure topology and edge states in one and two dimensions* (Springer, 2016).