

# Observable topological effects in molecular devices with Möbius topology

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We study the topological properties of quantum states for the spinless particle hopping in a Möbius ladder. This system can be regarded as a molecular device possibly engineered from the Möbius annulenes, which enjoys a pseudospin orbital interaction described by a non-Abelian gauge structure. It results from the nontrivial topology of configuration space and results in various observable effects, such as optical spectral splitting. The transmission spectrum through the Möbius molecular device is calculated to demonstrate a topological effect as destructive interferences in the conduction band. The induced interaction also leads to an entanglement between the transverse and longitudinal modes for any locally factorized state.

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## I. INTRODUCTION

With various potential applications, the molecular-based devices have motivated extensive experimental and theoretical investigations (see Ref. 1). The engineered molecular architectures display novel quantum effects. After the theoretical prediction of Möbius molecules in 1964,<sup>2</sup> various kinds of molecules and nanostructures with Möbius topology were synthesized<sup>3,4</sup> or designed.<sup>5,6</sup> With these significant developments of engineering topologically nontrivial structures, the topological properties of quantum systems become more and more important. Thus, it is natural to consider the various quantum effects induced by the nontrivial topological configurations,<sup>7-12</sup> such as the Möbius molecule.

For the topological effects in quantum mechanics, it is a fundamental principle (assumption) that the wave function must be single valued in a topologically trivial configuration. In this sense, various topological effects such as Aharonov-Bohm (AB) effect can be rationally explained without the introduction of any extra assumption in quantum mechanics.<sup>13</sup> In some configurations with nontrivial topological structure, although the motion of particle requires some complex boundary conditions, such topological nontrivialness of the configuration space can be canceled by introducing a singular gauge field. A typical example is the phenomena of persistent currents in a mesoscopic or a superconducting ring threaded by a magnetic flux. Here, the  $U(1)$  gauge field can be introduced to cancel the seemingly multivalued boundary condition with a nonintegrable AB phase factor. Another illustration is the fractional statistics of anyons, which describes the effective quantum excitations of the hard-core particles confined strictly in two dimensions with the braiding homotopy of the many-body configuration.<sup>14</sup>

In this paper, we show a topology-induced quantum effect with a non-Abelian gauge structure, which emerges from the twisted boundary condition in a Möbius ladder. The twisted boundary condition results in a local interaction between transverse and longitudinal modes. In the continuous limit, the spinless particle moving in the Möbius ladder is mapped to a pseudospin coupled to the orbit corresponding to the longitudinal mode. When we apply a transverse field, the

pseudospin seems to be confined in a one-dimensional ring and subject to a texturelike effective magnetic field, together with an effective magnetic flux threading the ring (see Fig. 1). Different from the existing setups of mesoscopic ring for persistent currents,<sup>15</sup> the effective magnetic flux in our molecular device depends on the pseudospin state, namely, there exists a non-Abelian gauge field induced by the Möbius topology.

Compared with the topologically trivial configurations, i.e., an ordinary tight binding ladder, the quantum state of the Möbius molecule is strongly affected by its configuration topology. Here, we predict three quantum interference effects, which are distinguished from the ordinary cases obviously: (i) the Stark effect in the electric field causes more optical spectral splitting due to the effective Zeeman effect by the induced non-Abelian gauge field, (ii) the transmission spectrum through the Möbius molecule is significantly modified due to the destructive interference caused by the non-Abelian flux, and (iii) from the view of quantum information, the entanglement is emerged from the locally factorized state in the Möbius molecule.

The paper is organized as follows. In Sec. II, the concept of topology-induced non-Abelian gauge structure is introduced. This concept helps us to establish the physical picture of the various topological effects predicted in Sec. III. Conclusions are given in Sec. IV.

## II. INDUCED NON-ABELIAN GAUGE STRUCTURE

Both experimental<sup>3,4</sup> and theoretical<sup>7-12</sup> investigations on the  $\pi$ -electron systems,<sup>2,6</sup> nonconjugated molecules,<sup>3</sup> and

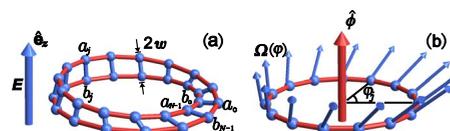


FIG. 1. (Color online) (a) Schematic illustration of Möbius ladder. (b) An electron hopping in the Möbius ladder can be mapped to a pseudospin moving in a one-dimensional ring with a spin-dependent flux  $\hat{\phi}$  and a texturelike inhomogeneous magnetic field  $\Omega(\varphi)$ .

even inorganic nanostructures made by NbSe<sub>3</sub> (Ref. 4) suggest that the electron moving in the Möbius systems can be described by a tight-binding model with a twisted ladder configuration illustrated in Fig. 1(a). Since there is no spin flip, the electron is regarded as a spinless particle. There are  $2N$  lattice sites, located at the two edges of the ladder, whose coordinates are

$$\mathbf{r}_{j\pm} = \left( \cos \varphi_j \tilde{R}_{\pm}(\varphi_j), \sin \varphi_j \tilde{R}_{\pm}(\varphi_j), \pm w \cos \frac{\varphi_j}{2} \right). \quad (1)$$

Here  $\tilde{R}_{\pm}(\varphi_j)$  is defined as  $\tilde{R}_{\pm}(\varphi_j) \equiv R \pm w \sin(\varphi_j/2)$  with half width  $w$  and “radius”  $R$  and  $\varphi_j = 2\pi j/N$  is the polar coordinate (see Fig. 1). We use operators  $a_j^\dagger$  ( $a_j$ ) and  $b_j^\dagger$  ( $b_j$ ) to denote the creating (annihilating) a particle on  $j$ th site of each edges, respectively. The rungs represent the coupling between  $a$  chain and  $b$  chain. We assume that the hopping strength along the ladder is homogeneous. Then the Hamiltonian reads

$$H = \sum_{j=0}^{N-1} \mathbf{A}_j^\dagger \mathbf{M}_j \mathbf{A}_j - \xi \sum_{j=0}^{N-1} (\mathbf{A}_j^\dagger \mathbf{A}_{j+1} + \text{H.c.}), \quad (2)$$

where  $\mathbf{A}_j = (a_j, b_j)^T$  and the matrix

$$\mathbf{M}_j = \begin{pmatrix} \varepsilon_j & -V_j \\ -V_j & -\varepsilon_j \end{pmatrix} = \varepsilon_j \sigma_z - V_j \sigma_x \quad (3)$$

for  $\sigma_{x,y,z}$  being the Pauli matrices with  $V_j$  representing the coupling strength between  $a$  and  $b$  sites and  $2\varepsilon_j$  describing the on-site energy difference, which could be induced by external electric field (see Sec. III).

The Möbius boundary conditions are  $a_N = b_0$  and  $b_N = a_0$  or, equivalently,  $\mathbf{A}_N = \sigma_x \mathbf{A}_0$ . It is this boundary condition that results in the interesting topological properties of the quantum state. In terms of the operator-valued vector

$$\mathbf{B}_j \equiv \begin{pmatrix} c_{j\uparrow} \\ c_{j\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\varphi_j/2} & -e^{-i\varphi_j/2} \\ 1 & 1 \end{pmatrix} \begin{pmatrix} a_j \\ b_j \end{pmatrix}, \quad (4)$$

which is a unitary transformation of  $\mathbf{A}_j$ , the Hamiltonian is rewritten as

$$H = \sum_{j=0}^{N-1} \mathbf{B}_j^\dagger (\boldsymbol{\Omega}_j \cdot \boldsymbol{\sigma}) \mathbf{B}_j - \xi \sum_{j=0}^{N-1} (\mathbf{B}_j^\dagger \mathbf{Q} \mathbf{B}_{j+1} + \text{H.c.}), \quad (5)$$

where

$$\boldsymbol{\Omega}_j \equiv \left( \varepsilon_j \cos \frac{\varphi_j}{2}, \varepsilon_j \sin \frac{\varphi_j}{2}, V_j \right)^T \quad (6)$$

is a direction vector and matrix  $\mathbf{Q}$  is defined as

$$\mathbf{Q} \equiv \begin{pmatrix} e^{i\pi/N} & 0 \\ 0 & 1 \end{pmatrix}. \quad (7)$$

It should be emphasized that the operator  $\mathbf{B}_j$  only requires the ordinary periodic boundary condition, i.e.,  $\mathbf{B}_N = \mathbf{B}_0$ . So far, we have shown that the nontrivial Möbius boundary condition is canceled by the unitary transformation, accompanied by an induced non-Abelian gauge field associated with

$\boldsymbol{\Omega}_j$  and  $\mathbf{Q}$ . This point will be seen more clearly in the continuous limit below.

In the continuous limit (i.e.,  $N \rightarrow \infty$  and  $\varphi_j \rightarrow \varphi \in [0, 2\pi]$ ), the particle hopping on a Möbius ladder is described by the two-component Hamiltonian (5), which can be mapped to the continuous Hamiltonian

$$H = \left( -i \frac{\partial}{\partial \varphi} - \hat{\phi} \right)^2 + \boldsymbol{\Omega}(\varphi) \cdot \boldsymbol{\sigma}. \quad (8)$$

This Hamiltonian (8) describes a pseudospin moving in a one-dimensional ring subject to non-Abelian gauge field including a spin-dependent flux arising from the matrix  $\mathbf{Q}$  in Eq. (7),

$$\hat{\phi} = \frac{1}{4}(\sigma_z + 1), \quad (9)$$

and an inhomogeneous magnetic field  $\boldsymbol{\Omega}(\varphi)$ . Here, the natural unit is chosen. In this sense, the induced magnetic flux  $\hat{\phi}$  is an operator, which does not commute with the Zeeman term  $\boldsymbol{\Omega} \cdot \boldsymbol{\sigma}$ , and the gauge field is called non-Abelian.

### III. TOPOLOGY-INDUCED EFFECTS

#### A. Topological Stark shift and spectral splitting

Now, we consider the Möbius molecule subject to a uniform electric field. First of all, let us consider the electric field  $\mathbf{E} = E_z \hat{\mathbf{e}}_z$  along the  $z$  direction [see Fig. 1(a)]. In this case, the electric-field-induced on-site energy difference is

$$2\varepsilon_j = \mathbf{E} \cdot (\mathbf{r}_{j+} - \mathbf{r}_{j-}) \equiv 2\varepsilon \cos\left(\frac{\varphi_j}{2}\right). \quad (10)$$

By assuming the homogeneous coupling  $V_j \equiv V$ , the effective magnetic field

$$\boldsymbol{\Omega}_j = \left( \frac{\varepsilon}{2}(1 + \cos \varphi_j), \frac{\varepsilon}{2} \sin \varphi_j, V \right)^T \quad (11)$$

possesses a texturelike distribution [Fig. 1(b)] with spatially varying amplitude and direction.

The Stark effect, i.e., the energy shift under the weak electric field, is calculated by the perturbation approach. For simplicity of notation, we present the result in the continuous limit. By taking the unperturbed Hamiltonian

$$H_0 = \left( -i \frac{\partial}{\partial \varphi} - \hat{\phi} \right)^2 + \Omega_z \sigma_z, \quad (12)$$

the zeroth-order eigenenergy is

$$E_{n\uparrow} = \left( n - \frac{1}{2} \right)^2 + V, \quad (13a)$$

$$E_{n\downarrow} = n^2 - V, \quad (13b)$$

and the corresponding eigenstates are denoted as  $|n, \chi\rangle = |n\rangle |\chi\rangle$  for  $\chi = \uparrow, \downarrow$  and

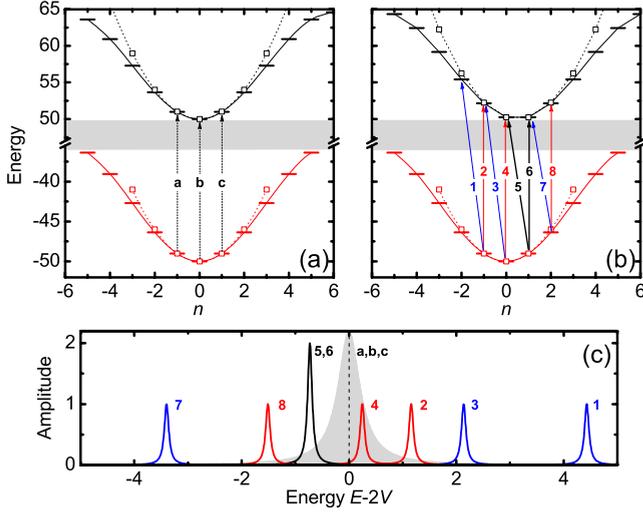


FIG. 2. (Color online) Energy levels (the solid lines with dash marks) for (a) the ordinary ring and (b) the Möbius ladder. The dotted lines with empty square marks are the energy levels in the continuous limit. The allowed transitions induced by a electric field in the  $z$  direction are depicted by the arrows. (c) The optical spectra of the Möbius ladder corresponding to the transitions shown in (b). The gray peak centered at the origin is the spectra for the ordinary ring. The Lorentz profile is assumed for each peak with phenomenological broadening. Parameters used in calculation are  $N=12$  and  $V=50$ .

$$\langle \varphi | n \rangle = \frac{1}{\sqrt{2\pi}} e^{in\varphi}. \quad (14)$$

The energy spectra of these unperturbed states, illustrated in Fig. 2(b) in comparison with the ordinary ring in Fig. 2(a), show the obvious spectral splitting.

The perturbation Hamiltonian

$$H' = \Omega_x(\varphi)\sigma_x + \Omega_y(\varphi)\sigma_y \quad (15)$$

results in the superposition of the zeroth-order states with different pseudospin components. The Stark shifts  $\delta E_{n\chi}$  under the static electric field are calculated as

$$\delta E_{n\uparrow} = \frac{\varepsilon^2(V-n-1/8)}{3n^2 - 8Vn + (4V^2 - V - 3/16)}, \quad (16a)$$

$$\delta E_{n\downarrow} = \frac{-\varepsilon^2(V-n+5/8)}{3n^2 - (8V+3)n + (4V^2 + 5V + 9/16)}. \quad (16b)$$

Together with the nonvanishing transition matrix elements

$$\langle n\uparrow | H' | n+1\downarrow \rangle = \langle n\uparrow | H' | n\downarrow \rangle = \frac{\varepsilon}{2}, \quad (17)$$

this energy shifts due to the twisted boundary condition are regarded as an observable quantum effect of the induced non-Abelian gauge field.

In view of the future experiments, the topology state of the Möbius molecule may be detected by the splitting of the optical spectra. We consider the transitions of the electron in the Möbius molecule under an optical excitation. We assume

that the molecules are subjected to the linearly polarized light, whose electric field component  $\mathbf{E}(t) = E_z(t)\hat{e}_z$  oscillates in the  $z$  direction. The time-dependent Hamiltonian is  $H(t) = H_0 + \tilde{H}'(t)$ , where the perturbation  $\tilde{H}'(t) = \mathbf{E}(t) \cdot \mathbf{r} = H' \cos \omega t$  with  $\omega$  being the frequency of the pumping light. The transition selection rules shown in Fig. 2 arise from the above-mentioned transition matrix elements as

- (i)  $|n\uparrow\rangle \rightleftharpoons |n\downarrow\rangle$ ,
- (ii)  $|n\uparrow\rangle \rightleftharpoons |n+1\downarrow\rangle$ . (18)

The Fermi golden rule is applied to calculate the spectra with various excitation energies. In comparison with the case of ordinary ring, where only one peak is located at frequency  $\hbar\omega = 2V$  since the only transition (i) is allowed in this case, the optical spectra of Möbius molecule show clear splitting due to the nontrivial topology.

Since the spectral lines are always taken from ensemble of molecules with random orientation, it is worth discussing the case of different electric field directions. For definiteness, let us consider the in-plane electric field in the  $x$  direction, i.e.,  $\mathbf{E} = E_x \hat{e}_x$  (similar analysis could be applied for  $\mathbf{E} = E_y \hat{e}_y$ ). In this case, the electric-field-induced on-site energy difference becomes

$$2\varepsilon_j = \mathbf{E} \cdot (\mathbf{r}_{j+} - \mathbf{r}_{j-}) \equiv 2\varepsilon \cos(\varphi_j) \sin\left(\frac{\varphi_j}{2}\right). \quad (19)$$

Thus, as discussed above, the effective magnetic field felt by the pseudospin is

$$\mathbf{\Omega}_j = \left( \frac{\varepsilon}{4} \sin 2\varphi_j, \frac{\varepsilon}{2} \cos \varphi_j (1 - \cos \varphi_j), V \right)^T. \quad (20)$$

This spatially inhomogeneous field, as a perturbation in Eq. (15), will introduce the coupling between the zeroth-order states  $|n\downarrow\rangle$  in the conduction band and  $|n'\uparrow\rangle$  in the conduction band ( $n$  and  $n'$  are integers) by the following transition matrix elements:

$$\begin{aligned} \langle n\uparrow | H' | n\downarrow \rangle &= \langle n-2\uparrow | H' | n\downarrow \rangle = \frac{i\varepsilon}{4}, \\ \langle n\pm 1\uparrow | H' | n\downarrow \rangle &= -\frac{i\varepsilon}{4}. \end{aligned} \quad (21)$$

Thus, under the oscillating electric field, the transition selection rules for the  $x$ -polarized electric field become

$$\begin{aligned} |n\downarrow\rangle &\rightleftharpoons |n\uparrow\rangle, \quad |n\downarrow\rangle \rightleftharpoons |n-2\uparrow\rangle, \\ |n\downarrow\rangle &\rightleftharpoons |n\pm 1\uparrow\rangle. \end{aligned} \quad (22)$$

Accordingly, there are *four* possible interband transitions under the in-plane electric field for the Möbius molecules. In contrast to the Möbius rings, the in-plane electric field *does not* induce any interband transitions for the ordinary ring, since, in this case, the electric-field-induced on-site energy difference vanishes, i.e.,  $2\varepsilon_j = \mathbf{E} \cdot (\mathbf{r}_{j+} - \mathbf{r}_{j-}) = 0$ , and then the transition matrix elements  $\langle n\uparrow | H' | n'\downarrow \rangle$  also vanish for the ordinary ring.

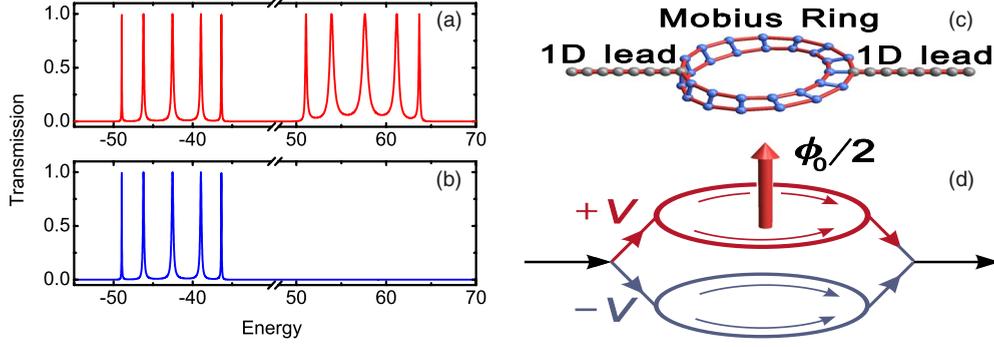


FIG. 3. (Color online) Transmission spectra for (a) the ordinary ring and (b) the Möbius ring. (c) Schematic illustration of the Möbius molecule joining with two leads. (d) Schematic illustration of the topology-induced magnetic flux in the conduction band (see text). The same parameters are used as in Fig. 2.

The ensemble measurement of the spectral line could be obtained by averaging the in-plane and perpendicular electric field cases. According to the analysis above, one can conclude that, compared with the ordinary rings, spectral line splitting occurs due to the nontrivial topology-induced gauge structure.

### B. Transmission through a Möbius ring

Besides the topology-induced Stark shift and the spectral splitting, the transmission through the Möbius ring exhibits obvious differences from the ordinary ring.<sup>12</sup> We consider a molecule connected to two leads as shown in Fig. 3(c). The leads are modeled by two semi-infinite chains. The electron can hop along the chains and tunnel between the leads and the Möbius ring. By assuming that the leads are connected with the ring at  $a_0$  and  $a_{N/2}$  sites, the Hamiltonians of the electron moving in the leads and its tunneling to the Möbius ring are written as

$$H_{\text{lead}} = t_l \sum_{k=1}^{\infty} c_{i,k}^\dagger c_{i,k+1} + \text{H.c.}, \quad (23)$$

$$H_{\text{tun}} = t_l (c_{R,1}^\dagger a_0 + c_{L,1}^\dagger a_{N/2}) + \text{H.c.}, \quad (24)$$

respectively, where  $c_{i,k}$  for  $i=L,R$  are the annihilation operators of the electron in the leads and  $t_l$  describes the electron hopping amplitude.

To analyze the transmission for a given injection energy  $E$ , we calculate the self-energies  $\Sigma_{L,R}$  to determine the Green's function of the Möbius ring,

$$G(E) = \frac{1}{E - H - \Sigma_L - \Sigma_R}, \quad (25)$$

by taking account of the influence of the semi-infinite leads.<sup>16</sup> The self-energies  $\Sigma_{L,R}$  can be obtained numerically and they give the level broadenings  $\Gamma_{L,R} = -2 \text{Im} \Sigma_{L,R}$ . The transmission coefficient  $T(E)$  is obtained by the relation<sup>16</sup>

$$T(E) = \text{Tr}[\Gamma_R G \Gamma_L G^\dagger]. \quad (26)$$

The transmission spectrum of the Möbius ring is shown in Fig. 3(b), comparing with that of the ordinary mesoscopic

ring with periodic boundary conditions [Fig. 3(a)]. For simplicity,  $\varepsilon_j=0$  and  $V_j=V$  are assumed. Through the unitary transformation from  $\mathbf{A}_j$  to  $\mathbf{B}_j$ , the Möbius ladder is decomposed into two independent rings (channels) [see Fig. 3(d)]. In the strong-coupling limit, i.e.,  $V \gg \xi$ , the energy spectrum of the channels is split into two bands. The energy gap between them is determined by the coupling strength  $V$ . Below the energy gap (or in the “valence band”), the transmission behaviors are locally similar in both cases. It is not affected by the topology of configuration space since, as discussed before, the induced gauge field is not present in the valence-band channels. Above the energy gap (or in the “conduction band”), the transmission coefficient is completely suppressed in the Möbius ring due to the induced gauge field, which equals to a half magnetic flux quanta. The particle could not transmit through the Möbius ring at such energies due to the destructive interference between the two arms of the ring.

It is interesting to mention that either the left lead connected to the molecule at the  $a_{N/2}$  site or the  $b_{N/2}$  site does not affect the result in Fig. 3(b), i.e., the suppression of the transmission in the conduction band. This can be understood by the following argument. In the decoupled representation [see Fig. 4(c)], when the left lead is connected with  $a_{N/2}$  site as in Fig. 4(a), the tunneling between the left lead and the molecule is written as

$$H_{\text{tun}}^{L,a} = t_l c_{L,1}^\dagger a_{N/2} + \text{H.c.} \equiv t_{L,a}^c c_{L,1}^\dagger c_{N/2\uparrow} + t_{L,a}^v c_{L,1}^\dagger c_{N/2\downarrow} + \text{H.c.}, \quad (27)$$

where, according to transformation (4) and the Hamiltonian (24), the tunneling amplitude to the conduction band  $t_{L,a}^c = -it_l/\sqrt{2}$ . In the case of Fig. 4(b), one can check that the

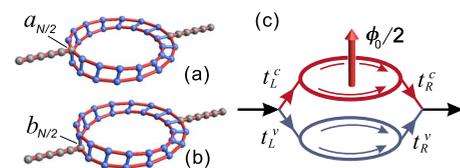


FIG. 4. (Color online) The left lead connected to the molecule at the site  $a_{N/2}$  in (a) and  $b_{N/2}$  in (b). (c) Schematic illustration of the tunneling amplitudes from the left (right) lead to the conduction (valence) channel.

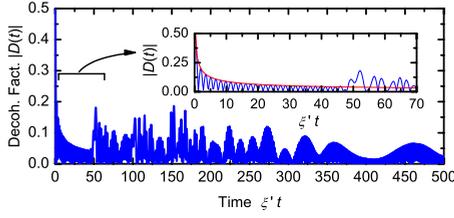


FIG. 5. (Color online) The decoherence factor as a function of time. Inset: detailed behavior of the decoherence factor and its asymptotic envelope for small  $t$ .  $N=50$  is assumed.

tunneling amplitude to the conduction band is different by a factor of  $-1$ , i.e.,  $t_{L,b}^c = it_l/\sqrt{2}$ . So we conclude that the connection of left lead to the  $a_{N/2}$  or  $b_{N/2}$  site does not affect the relative phase between the two ring arms in the conduction band. Thus, in both cases shown in Figs. 4(a) and 4(b), the destructive interference condition in the conduction band is unchanged. In other words, the suppression of the transmission in the conduction band induced by the Möbius structure will occur for both cases.

### C. Decoherence from induced Stern-Gerlach effect of pseudospin

The third topological phenomenon is the quantum decoherence (Fig. 5) of the pseudospin caused by the Stern-Gerlach effect of the induced gauge field.<sup>17</sup> Actually, through the spin-orbit coupling, quantum entanglement between different spin states is created, so that a quantum measurement can be realized. Similar to the Stern-Gerlach experiment, the spatial degrees of freedom interacts with spin in a nondemolition fashion and thus measures the spin states. Here, we point out that the situation may be different from the topologically nontrivial case without obvious local coupling. We have shown that the gauge field can be induced by the Möbius boundary condition, and the effective pseudospin orbital interaction further arises from this gauge field. Thus, the entanglement could be created by the topology-induced effect in the absence of any *real* local interactions.

In order to emphasize the main physical mechanism in our argument, we assume the homogeneous conditions  $\varepsilon_j = 0$  and  $V_j = V$ . Thus, only the  $\sigma_z$  component is retained and thus Hamiltonian (5) is of a block-diagonal form, i.e.,  $H = \text{diag}[H_\uparrow, H_\downarrow]$  with the conditional Hamiltonians

$$H_\chi = \pm V \sum_{j=0}^{N-1} c_{j\chi}^\dagger c_{j\chi} - \sum_{j=0}^{N-1} (\xi_\chi c_{j\chi}^\dagger c_{j+1\chi} + \text{H.c.}), \quad (28)$$

where  $\chi \in \{\uparrow, \downarrow\}$ ,  $\xi_\uparrow = \xi$ , and  $\xi_\downarrow = \xi \exp(i\pi/N)$ .

We assume that one electron is initially located at the  $a_0$  site, i.e.,

$$|\psi(0)\rangle = a_0^\dagger |\text{vac}\rangle = \frac{1}{\sqrt{2}} |j=0\rangle \otimes (|\uparrow\rangle + |\downarrow\rangle). \quad (29)$$

In the pseudospin representation, this initial state stands for a pseudospin pointing in the  $x$  direction at the  $j=0$  site. Obviously, it is a locally factorized state. At time  $t$ , the wave function evolves into a superposition

$$|\psi(t)\rangle = \frac{1}{\sqrt{2}} (|\psi_+(t)\rangle |\uparrow\rangle + |\psi_-(t)\rangle |\downarrow\rangle), \quad (30)$$

where the states

$$|\psi_\pm(t)\rangle = e^{-iH_\pm t} |j=0\rangle \quad (31)$$

can be understood as the *detector states* measuring the pseudospin states. As the so-called decoherence factor, the overlap

$$D(t) = \langle \psi_-(t) | \psi_+(t) \rangle = \frac{1}{2} \sum_{j=0}^{N-1} G_-^*(j,t) G_+(j,t) \quad (32)$$

of  $|\psi_\pm(t)\rangle$  characterizes the quantum coherence of pseudospin states. Here,

$$G_\pm(j,t) \equiv \langle j | \psi_\pm(t) \rangle = \sum_{k=-\infty}^{+\infty} e^{i\varphi_\pm(j_k)} J_{j_k}(2\xi t) \quad (33)$$

are the propagators of the two spin components, where  $J_n(x)$  is the  $n$ th order Bessel function. Here,  $j_k = j + kN$  represents the  $j$ th site with winding number  $k$  with respect to the two decomposed rings, and the two pseudospin-dependent phases  $\varphi_+(j_k) = j_k \pi/2$  and  $\varphi_-(j_k) = \varphi_+(j_k) + j_k \pi/N$  accompany the longitudinal motions in the two rings. It is the induced phase shift  $j_k \pi/N$  between  $\varphi_\pm(j_k)$  that gives rise to the decoherence of pseudospin. Straightforwardly, the decoherence factor is calculated as

$$D(t) = \frac{1}{2} e^{2iVt} \sum_{\delta=-\infty}^{\infty} i^\delta J_{\delta N}(2\xi' t), \quad (34)$$

where  $\xi'$  is defined as

$$\xi' = \xi \sqrt{2 - 2 \cos(\pi/N)}. \quad (35)$$

It is clear that, in the limit with large  $N$ , the short-time behaviors of the decoherence factor is dominated by only one term with  $\delta=0$ ; thus, the decoherence factor

$$|D(t)| \approx |J_0(2\xi' t)| \quad (36)$$

with a time-dependent envelop  $\sqrt{N/(2\pi\xi' t)}$  decaying as inverse square root of time.

## IV. CONCLUSION

Taking the Möbius ladder as an illustration, we have explored the role of topological structure of the configuration space on the quantum states of the particles confined in a topologically nontrivial manifold. The global properties of the topological system can be locally described by a non-Abelian gauge structure, which can result in some observable effects in the aspects of spectroscopy, such as the topologically induced Zeeman splits and the higher-energy band suppression of the transmission of the Möbius molecule. We also show the quantum decoherence of the pseudospin and the entanglement due to the pseudospin orbital interaction.

The theoretical model proposed in this paper could be used to describe the underlying physics in various kinds of structure with Möbius structure, including the organic mol-

ecules, inorganic structures, and artificial quantum systems. It is possible to observe the predicted nontrivial topological phenomena in these kinds of systems. Particularly, in the view of chemistry, these observable effects can be regarded as the physical signals of the successful synthesis of some Möbius aromaticity molecules. These methods may be used to distinguish the topologically nontrivial molecules from the ordinary ones.

## ACKNOWLEDGMENTS

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