Witness of topological phase transition and Weyl points in an open topological system

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Recently, the tunable Weyl-semimetal bands and the associate topological phase transition have been successfully simulated in superconducting quantum circuits [X. Tan, et al. Phys. Rev. Lett. 122, 010501 (2019)]. Since the superconducting quantum circuits inevitably couple to the environment, we here focus on the steady state and decoherence process by taking the reservoir into consideration via quantum master equation. Our results show that the purity of the steady state can be used to indicate the topological phase transition and Weyl points. Furthermore, the coherence will exponentially decay to zero at the Weyl points, and decay to a nonzero value with oscillation at other points in the momentum space. Our work may have significant impact on the study of quantum open topological system.

I. INTRODUCTION

Topological effects in electronic [1–7] and photonic system [8–13] have attracted broad attentions for both of the understanding of fundamental physics and possible realization of robust quantum information processing [14–16]. Due to the limited flexibility of engineering and manipulating the electronic system, people have designed many photonic structures to simulate the phenomenon associated with topological phase transition.

Among the various topological materials, Weyl semimetal represents a novel family [17–19]. It can be described by a two-band model, and the upper and lower energy bands will contact each other at the Weyl points as the system undergoes the topological phase transition. In Sec. II, we discuss the purity of the steady state and demonstrate the trajectories of the steady state in the Bloch representation as the system undergoes the topological phase transition. In Sec. IV we illustrate the decoherence process. Finally, we end up with a brief conclusion in Sec. V.

II. MODEL AND STEADY STATE

A. Hamiltonian

A Weyl-semimetal Hamiltonian in the simulation by superconducting quantum circuits [20] can be simply written as

$$H = \sin k_x \sigma_x + \sin k_y \sigma_y + (\lambda + \cos k_z) \sigma_z + u_0(k) \sigma_0,$$

where $\sigma_x, \sigma_y, \sigma_z$ are the Pauli matrices and $\sigma_0$ is the unit matrix. $k = (k_x, k_y, k_z)$ is the wave vector. $\lambda (|\lambda| \leq 1)$ is an experimentally controllable parameter. In most cases, $u_0(k)$ is zero or a $k$-independent constant and we set $u_0 = 0$ in what follows. The Hamiltonian in Eq. (1) actually corresponds to a two-band physical model. For any given wave vector $k$, it describes the Hamiltonian of a two-level system moving in an effective magnetic field. That is, $H = \vec{B} \cdot \vec{\sigma}$ with $\vec{B} = (\sin k_x, \sin k_y, \lambda + \cos k_z)$ and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. In the simulation of topological bands [20], the effective magnetic field is realized by the on-demand microwave driving fields. The energy spectrum of the Hamiltonian can be obtained as

$$E_{\pm} = \pm \sqrt{(\lambda + \cos k_z)^2 + (\sin^2 k_x + \sin^2 k_y)}$$

which satisfies $E_{+} = -E_{-}$. Moreover, it is obvious that

$$\min_{(k_x, k_y)} E_{+} = |\lambda + \cos k_z|, \max_{(k_x, k_y)} E_{-} = -|\lambda + \cos k_z|. \tag{3}$$
As a result, the upper and lower energy bands will only contact each other when \( \lambda + \cos k_z = 0 \).

In Fig. 1 we plot the energy spectrum as functions of the wave vectors \( k_x \) and \( k_y \) in the first Brillouin zone, that is, \( k_x \in (-\pi, \pi], k_y \in (-\pi, \pi] \). Choosing the parameters \( \lambda = 0, k_z = \pi/2 \), we show that the upper band \( E_+ \) and the lower band \( E_- \) will touch at four points with \( (k_x, k_y) = (0, 0), (k_x, k_y) = (\pi, 0), (k_x, k_y) = (0, \pi) \) and \( (k_x, k_y) = (\pi, \pi) \) in Fig. 1(a). These points, which are the signatures of semimetal, are named as Weyl points in electronic system. At these Weyl points, the gap between the two bands will be closed and reopened as the system undergoes topological phase transition, that is, the parameter \( \lambda + \cos k_z \) changes its sign from negative (positive) to positive (negative). As a result, \( \lambda + \cos k_z = 0 \) is the critical point for the topological phase transition. In addition, we also observe that \( E_+ \) will achieve its maximum value at another four points with \( (k_x, k_y) = (\pm \pi/2, \pm \pi/2) \) in Fig. 1(b). In what follows of this paper, we will name them as “anti-Weyl” points.

B. Master equation and steady state

Recently, the topological bands have been simulated in the quantum superconducting circuits \([31, 34]\), where a three-dimension transmon qubit serves as two-level or three-level system. In this sense, one can manipulate the system by adjusting the pump microwave artificially, which is more accessible than the operations in electronic system. However, the transmon qubits can never be isolated from the surrounding environments. As a result, we need to regard the system as a quantum open system and the dynamics is governed by the master equation

\[
\frac{d\rho}{dt} = -i [H, \rho] + \frac{\gamma}{2} \left( 2\sigma_- \rho \sigma_+ - \sigma_+ \sigma_- \rho - \rho \sigma_+ \sigma_- \right),
\]

where \( \rho \) is the density matrix of the system, \( \sigma^\pm = (\sigma_x \pm i \sigma_y)/2 \) and \( \gamma \) is the decay rate, which characterizes the coupling strength between the system and the environments. In the rest of this paper, we set all of the parameters to be dimensionless.

In the basis of \( \{|e\}, \{|g\}\} \), where \( \sigma_z |e\rangle = +(-)|e\rangle \), the steady state \( \langle d\rho_{ss}/dt = 0 \rangle \) can be obtained as

\[
\rho_{ss} = \begin{pmatrix}
\rho_{ee} & \rho_{eg} \\
\rho_{ge} & 1 - \rho_{ee}
\end{pmatrix},
\]

where \( \rho_{gg} = 1 - \rho_{ee} \) and

\[
\rho_{eg} = \frac{-[4 (\lambda + \cos k_z) + i \gamma] (\sin k_x - i \sin k_y)}{4 (\sin^2 k_x + \sin^2 k_y) + 8 (\lambda + \cos k_z)^2 + \frac{\gamma^2}{4}},
\]

\[
\rho_{ee} = \frac{2 (\sin^2 k_x + \sin^2 k_y)}{4 (\sin^2 k_x + \sin^2 k_y) + 8 (\lambda + \cos k_z)^2 + \frac{\gamma^2}{4}}.
\]

III. PURITY AND BLOCH SPHERE REPRESENTATION

In the last section, we have obtained the steady state of a semimetal system when it is subject to the surrounding environments. Due to the dissipation and decoherence induced by the environment, we will usually get a mixed steady state. To characterize how “mixed” of the steady state, we here investigate the behavior of purity \( P = \text{Tr} \rho_{ss}^2 \) for different \( k_x \) and \( k_y \). A direct calculation based on Eq. (5) yields

\[
P = 1 + 2 \left( |\rho_{eg}|^2 - \rho_{ee} \rho_{gg} \right).
\]

This expression suggests that the purity, i.e., the value of \( P \), is determined by the competition between the coherence \( \rho_{eg} \) and the populations \( \rho_{ee} \) and \( \rho_{gg} \). The coherence contributes positively to purity (the term \( |\rho_{eg}|^2 \)) and the populations contribute negatively to purity (the term \( -\rho_{ee} \rho_{gg} \)). Since all of the eigen values of a physical density matrix should be between 0 and 1, we readily
have $0 \leq \rho_{ee}\rho_{gg} - |\rho_{eg}|^2 \leq 1/4$. Only when the coherence matches the populations by $|\rho_{eg}|^2 = \rho_{ee}\rho_{gg}$, we will achieve $P = 1$, which implies the steady state is a pure state. Meanwhile, when $\rho_{ee}\rho_{gg} - |\rho_{eg}|^2 = 1/4$, we will have $P = 1/2$, corresponding to a fully mixed steady state.

Combining Eqs. (6) and (7), the purity can be explicitly expressed as

$$P = 1 - 8 \left[ \frac{\sin^2 k_x + \sin^2 k_y}{4(\sin^2 k_x + \sin^2 k_y) + 8(\lambda + \cos k_x)^2 + \gamma^2/2} \right]^2.$$  

(8)

First, for an arbitrary value of $\lambda + \cos k_z$, the purity reaches its maximum value at the Weyl points with $\sin k_x = \sin k_y = 0$ and minimum value at the anti-Weyl points satisfying $\sin^2 k_x + \sin^2 k_y = 2$. By choosing the topological phase transition point ($\lambda + \cos k_z = 0$), we plot the purity as functions of $k_x$ and $k_y$ in Fig. 2(a).

The results show that the purity behaves similarly to the energy spectrum in the momentum space. Therefore, the purity can be used to indicate the Weyl points in open semimetal system. Second, for an arbitrary fixed point other than $k_x = k_y = 0$ in the momentum space, as shown in Fig. 2(b), the purity exhibits as a nonmonotonic function of $\lambda + \cos k_z$ and achieves its minimum value at the topological phase transition point. It implies that, the purity of steady state can also be served as a signature of the phase transition.

It is interesting to investigate the steady state at the topological phase transition point where $\lambda + \cos k_z = 0$. At any of four Weyl points as discussed in Sec. III, the dynamics of the system is only governed by the dissipation ($H = 0$) and the steady state is the pure state $|y\rangle$. On the contrary, at the anti-Weyl points, taking the point $(k_x, k_y) = (\pi/2, \pi/2)$ as an example, the density state of the steady state can be obtained as

$$\rho_{ss} = \frac{1}{16 + \gamma^2} \begin{pmatrix} 8 & -2\gamma(1 + i) \\ -2\gamma(1 - i) & 8 + \gamma^2 \end{pmatrix},$$  

(9)

which becomes a fully mixed state in the limit of $\gamma \to 0$.

The steady state can also be illustrated geometrically on the Bloch sphere. In the Bloch representation, any quantum state of a qubit (two-level system) is indicated by a point with the position $R_i = \langle \sigma_i \rangle = \text{Tr}(\sigma_i \rho)$ ($i = x, y, z$), and the Bloch radius which characterizes its distance to the sphere center is $R = \sqrt{R_x^2 + R_y^2 + R_z^2}$.

In Fig. 2(c), we have demonstrated the trajectories as shown by the arrows as the parameter $\lambda + \cos k_z$ travels from $-2$ to $2$. Here the red solid spheres are for the anti-Weyl point with $k_x = k_y = \pi/2$, while the green triangles are those for $k_x = k_y = \pi/4$. It is obvious that the steady state at the topological phase transition point, which is represented by the big sphere or triangle respectively, has a smallest distance away from center of the Bloch sphere. This fact can also be revealed by connecting the Bloch radius to the purity via $R = \sqrt{2P - 1}$, which shows that $R$ is monotonously dependent of the
purity. Therefore, $R$ achieves its minimum value at the topological phase transition point, in consistent with the results in Fig. 3(b).

IV. DECOHERENCE

In the last section, we have shown that the purity of the steady state can witness the topological phase transition and the Weyl points in open semimetal system. Here, we will furthermore investigate the dynamical evolution, to study the decoherence process of the system.

Based on the master equation in Eq. (4), we will have the dynamical equation

$$
\frac{d\rho_{ee}}{dt} = i(\sin k_x + i \sin k_y)\rho_{eg} - i(\sin k_x - i \sin k_y)\rho_{eg}^* - \gamma \rho_{ee},
$$

and

$$
\frac{d\rho_{eg}}{dt} = (i \sin k_x + \sin k_y)(2\rho_{ee} - 1) - 2i(\lambda + \cos k_x) + \frac{\gamma}{2}\rho_{eg}.
$$

We prepare the system initially in a coherent superposition state $|\psi(0)\rangle = (|e\rangle + |g\rangle)/\sqrt{2}$, and plot the coherence $|\rho_{eg}|$ as a function of the evolution time $t$ for different $k_x$ and $k_y$ at the topological phase transition point $\lambda + \cos k_x = 0$ in Fig. 3. For the Weyl point ($k_x = k_y = 0$), the coherence undergoes an exponential decay, and finally disappears. In this case, the dynamics of the system is governed by the master equation

$$
\frac{d\rho}{dt} = \gamma \left(2\sigma_- \rho \sigma_+ - \sigma_+ \sigma_- \rho - \rho \sigma_+ \sigma_-\right),
$$

in which the decoherence is accompanied by the dissipation process. For the anti-Weyl point $k_x = k_y = \pi/2$, the dynamics is governed by

$$
\frac{d\rho}{dt} = -i[H, \rho] + \gamma \left(2\sigma_- \rho \sigma_+ - \sigma_+ \sigma_- \rho - \rho \sigma_+ \sigma_-\right),
$$

where the Hamiltonian

$$
H = \sigma_x + \sigma_y
$$

serves as a coherent driving. In this situation, the system is subject to the effective driving and dissipation simultaneously. Therefore, as shown in Fig. 4 the coherence undergoes the oscillations and then tends to be a nonzero constant, after the system reaches the steady state.

The time evolution of the quantum state can also be demonstrated in the Bloch representation. As shown in Fig. 4 preparing the initial state as $|\psi(0)\rangle = (|e\rangle + |g\rangle)/\sqrt{2}$, we track the trajectories of quantum state at Weyl and anti-Weyl points, respectively. In this process, we have shown how the initial coherent superposition state evolve into the ground state at the Weyl point ($k_x = k_y = 0$) and non-ground steady state at anti-Weyl point ($k_x = k_y = \pi/2$). Especially, for the anti-Weyl point, we clearly observe that the Bloch radius for the steady state is much smaller at the topological phase transition point [shown in Fig. 4(h)] compared with other situations, for example $\lambda + \cos k_x = 1$ as shown in Fig. 4(d), in consistency with the discussion about the steady state, as shown in the last section.

V. CONCLUSION

In summary, we have investigated the steady state and dynamical evolution process in an open semimetal system. For the steady state, our results show that the purity can be served as a indicator for the Weyl points and topological phase transition. At the Weyl points, the steady state of the system is exactly the ground state. At the other points in the momentum space, the purity of the steady state will achieve its minimum value as the
physical parameters go across the critical point of the topological phase transition (for the point of $k_x \neq k_y$, this fact is also true, but we did not show it in the previous discussions). Furthermore, the dynamical evolution of the coherence shows an exponential decay at the Weyl points while the decay exhibits some oscillations due to the effective driving at the other points in the momentum space. Therefore, the dynamical process also provides an approach to witness the Weyl points.

Recently, the topological band structure of the semimetal system has been simulated in superconducting quantum circuits, where the quantum state can be recovered by tomography technology\cite{36}. Therefore, we also illustrate the quantum state in the Bloch representation, and connect Bloch radius of the steady state to its purity. Our work combines the study of topological semimetal and the quantum open system, and we hope our study will stimulate the researches on quantum information process based on open topological system.

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