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Phase transitions in three-dimensional Dirac semimetal induced by off-resonant circularly polarized light

Pei-Hao Fu, Hou-Jian Duan, Rui-Qiang Wang, Hao Chen

Laboratory of Quantum Engineering and Quantum Materials, School of Physics and Telecommunication Engineering, South China Normal University, Guangzhou 510006, China

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A B S T R A C T

Three-dimensional Dirac semimetal is an ideal platform in studying topological phase transitions due to its exotic electronic structure. Based on the effective Hamiltonian of material Na_3Bi where two degenerated Dirac points are constructed by four Weyl nodes and protected by crystal symmetry, we study its Floquet phase transitions induced by circularly polarized light in off-resonant limit. By breaking the time-reversal symmetry and taking the quadratic momentum into account, abundant phases are realized, including Weyl semimetal, spin-polarized Weyl semimetal (SP-WSM), and normal insulator. The SP-WSM phase is a new phase, in which only pairs of spin-up (or spin-down) opposite-chirality Weyl nodes are remained while the other pairs of spin-down (or spin-up) opposite-chirality Weyl nodes are eliminated. Importantly, all the phase transitions can be manipulated not only by tuning the light intensity but also by changing the incident direction of light. To understand them, we have in detail analyzed the trajectory of Weyl nodes in $\mathbf{k}$ space controlled by the circularly polarized light and manifested them with the angle- and spin- dependent Hall conductivity.

1. Introduction

Recently, with the development of topological materials in the past decades, topological semimetals [4–12] are attaching more and more attention. Different from topological insulators [1–3], whose non-trivial gapless edge or surface states are topologically protected by the gapped bulk state, topological semimetals still supports robust metallic surface states even without gapped bulk states. As a three-dimensional (3D) counterpart of graphene, Dirac semimetals [9–11] (DSMs) possess closed points between conduction and valance bands in the bulk band. Around these band touching points, the low-energy dispersion can be captured by massless Dirac equation. The distinct electronic structure of the DSMs exhibits various interesting properties, such as the giant diamagnetism [13,14], negative magnetoresistance [15,16], and oscillating quantum spin Hall effect in quantum well structures [17]. Moreover, every single Dirac points in DSMs is composed of two Weyl points with opposite chirality. This feature makes the DSMs located at the phase boundary and suggests a flexible tunability in topological phases by symmetry breaking. Thus, the 3D DSM model can act as an ideal platform for studying topological phase transition [9,10].

One of powerful approaches to realize phase transition is irradiating off-resonant light to materials. In off-resonant region, electronic structure is modified through virtual photon processes instead of absorbing or emitting photons directly [18,19]. Such a processes usually leads two distinct effects, i.e. broking the time-reversal symmetry and renormalizing the Dirac mass term. As a result, the non-equilibrium systems can be approximately captured by an equilibrium one described by a new effective static Hamiltonian. These irradiated systems with new Hamiltonian are topologically distinct from the non-irradiated ones, which accounts for light-induced phase transitions [20]. There are extensively studies on this field [18–38]. In two-dimensional systems, irradiating high frequency light can shift Dirac nodes in graphene along with a transition between semimetallic and insulating phase [21,22]. In parallel with the study on graphene, phase transition concerning topological insulators also draws attentions, such as various phases realized in silecene [23,24] due to the competition between external electric field and circular polarized light. On the other hand, topological insulators can be realized from normal insulator [25], semiconductor quantum wells [26] and graphene [27,28] under high frequency driving, which gives rise to the Floquet chiral edge states and manipulates the topological properties of the bulk bands. Another topological phase transition in two dimensional

E-mail addresses: rqwanggz@163.com (R.-Q. Wang), chenhao@scnu.edu.cn (H. Chen).

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systems is realizing quantum anomalous Hall phase from either a quantum spin Hall phase or a trivial insulator phase by an off-resonant circularly polarized light, which acts effectively as a tunable Zeeman exchange field and an additional spin-dependent Dirac mass term [29]. As for three dimensional materials, realizing Floquet–Weyl semimetals by means of light becomes a focus. Many works have recently reported that Weyl semimetals (WSM) can be obtained from other topological materials, such as 3D magnetic topological insulator [19], stacked graphene systems [30], three-dimensional network model [31] and nodal line semimetal [32–35]. Also, when a beam of circularly polarized light is irradiated to DSMs [36–38], the degenerate Dirac nodes is split to Floquet–Weyl nodes by breaking time-reversal symmetry. The light-induced phase transitions can be verified by the non-zero anomalous Hall conductivity.

In this paper, we have studied the phase transitions of the DSM under the application of off-resonant light. The recent literatures [37,38] has realized the WSM from 3D DSM in the linear dispersion regime. We here take the quadratic terms of momentum into account and find that more abundant phases, including DSM, WSM, spin-polarized Weyl (SP-WSM) and normal insulator (NI), can be realized. More interestingly, the phase transition can be realized not only by tuning the intensity of light but also by changing the direction of incident light. This paper is organized as follows. The Floquet method and the corresponding effective Hamiltonian of the DSM is introduced in Sec. 2. Then, in Sec. 3, we analyze the photo-induced phase transitions, which can be realized by tuning the intensity or the direction of incident light. Discussions and summary are drawn in the final section.

2. Model and method

We begin with the effect model of Na_3Bi in the basis of $\left(\left|S^+_{1/2},\frac{1}{2}\right\rangle,\left|P^-_{3/2},\frac{3}{2}\right\rangle,\left|S^+_{1/2},-\frac{1}{2}\right\rangle,\left|P^-_{3/2},-\frac{3}{2}\right\rangle\right)$ as follows [9,36],

$$H(\boldsymbol{k})=\begin{pmatrix} H_+(\boldsymbol{k}) & B^*(\boldsymbol{k}) \\ B(\boldsymbol{k}) & H_-(\boldsymbol{k}) \end{pmatrix} \tag{1}$$

where $H_s(\boldsymbol{k})=\varepsilon_0(\boldsymbol{k})\tau_0+v_0\left(sk_x\tau_x-k_y\tau_y\right)+M(\boldsymbol{k})\tau_z$ with $\varepsilon_0(\boldsymbol{k})=C_0+C_1k_z^2+C_2\left(k_x^2+k_y^2\right)$ and $M(\boldsymbol{k})=M_0-M_1k_z^2-M_2\left(k_x^2+k_y^2\right)$. C_i, M_i, and v_0 are material dependent parameters, τ_0 and $\tau_{x,y,z}$ are unit matrix and Pauli matrixes for pseudospin and $s=+(-)$ denote for spin up (down). $B(\boldsymbol{k})$ is the high-order terms and in the threefold rotational symmetry it can be neglected. In our discussions, we set $B(\boldsymbol{k})=0$ since we concentrate on the behaviors in the vicinity of Dirac points. The first term $\varepsilon_0(\boldsymbol{k})$ in $H_s(\boldsymbol{k})$ breaks the electron–hole symmetry and M_0 in the last term acts as the Dirac mass. In Na_3Bi, the condition of $M_0/M_1>0$ leads the material to be DSM where one can obtain two Dirac nodes located at $\left(0,0,\pm\sqrt{M_0/M_1}\right)$, respectively. Each single Dirac node contains two Weyl nodes but with the net vanished chirality by mixing the spin-up and -down states. If the time reversal symmetry or inversion symmetry is broken, two Weyl nodes could be split with opposite chirality and DSM material naturally evolves into WSM. This behavior makes Na_3Bi become an attractive research platform for the topological transition.

In this paper, we consider a beam of off-resonant circularly polarized light (CPL) irradiated in k_x–k_z plane, as shown in Fig. 1. The azimuth angle θ measured from k_z-axis describes the direction of the light irradiation. This CPL can be modeled as a time-dependent vector potential

$$\boldsymbol{A}(t)=A_0\left(\cos\theta\cos\omega t,\eta\sin\omega t,-\sin\theta\cos\omega t\right) \tag{2}$$

where A_0 is the light intensity, ω is the frequency of light and $\eta=+(-)$ represents the right (left)-handed CPL. By Peierls substitution, $\boldsymbol{k}\to\boldsymbol{k}+\boldsymbol{A}(t)$, the Hamiltonian becomes time-dependent,

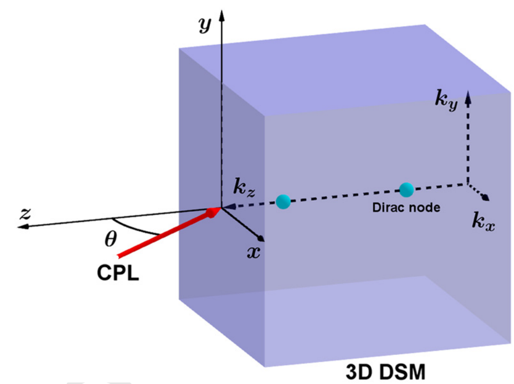

Fig. 1. Schematic diagram for an circularly polarized light (CPL) irradiated to a three-dimensional Dirac semimetal (3D DSM) with two Dirac nodes alone k_z and the incident azimuth angle θ measured from k_z-axis in k_x–k_z plane.

satisfying the periodic condition $H(\boldsymbol{k},t)=H(\boldsymbol{k},t+T)$ with period $T=2\pi/\omega$. Based on the Floquet theory [39–42], this periodic Hamiltonian can be expanded in Fourier series as $H(\boldsymbol{k},t)=\sum_n H_n(\boldsymbol{k})e^{in\omega t}$. In the off-resonant limit $A_0^2/\omega\ll 1$, one can decouple the zero-photon state from the other states and only consider its dressed effect through virtual photon absorption and emission processes [18,19]. As a consequence, the dressed electronic system is described in terms of an effective static Hamiltonian [18,36]

$$H'(\boldsymbol{k})=H_0(\boldsymbol{k})+\sum_{n=1,2}\frac{1}{n\omega}\left[H_{+n}(\boldsymbol{k}),H_{-n}(\boldsymbol{k})\right]+\hat{O}\left(1/\omega^2\right) \tag{3}$$

where $H_n(\boldsymbol{k})=\frac{1}{T}\int_0^T dt\,H(\boldsymbol{k},t)\,e^{-in\omega t}$ are the Fourier components of the time-periodic Hamiltonian. The renormalized Hamiltonian reads

$$H'_s(\boldsymbol{k})=H_s(\boldsymbol{k})+v'_0\left(sk_x\tau_x-k_y\tau_y\right)+M'_0\tau_z+\lambda k_z\tau_x \tag{4}$$

with

$$v'_0=s\eta\frac{2M_2A_0^2\cos\theta}{\omega}v_0$$
$$M'_0=s\eta\frac{v_0^2A_0^2\cos\theta}{\omega}-\frac{M_1A_0^2\sin^2\theta}{2}-\frac{M_2A_0^2\left(\cos^2\theta+1\right)}{2}$$
$$\lambda=-\eta\frac{2M_1A_0^2\sin\theta}{\omega}v_0.$$

The corresponding energy spectrum is

$$E^s_{\pm}(\boldsymbol{k})=\pm\sqrt{\left(svk_x+\lambda k_z\right)^2+v^2k_y^2+\left[M(k)+M'_0\right]^2} \tag{5}$$

where $v=v_0+v'_0$ and $\varepsilon_0(\boldsymbol{k})$ is ignored first for the convenience of discussions and will be specified later.

Compared the renormalized Hamiltonian in Eq. (4) with the unperturbed one in Eq. (1), we find there are three modified terms induced by the light field. The Fermi velocity around the Weyl nodes is changed by adding a spin-dependent term v'_0. Another is the revised Dirac mass term M'_0. It is worth mentioning that there is a spin relevant term $s\eta v_0^2A_0^2\cos\theta/\omega$ in M'_0, which displays an important role in splitting the spin degenerated bands and gives the DSM an opportunity to undergo much more abundant phase transitions. The last term in Eq. (4) couples k_z to the pseudospin component τ_x, and thus moves the position of the Weyl nodes from k_z axis to k_z–k_x plane.

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