Simulation of nodal-line semimetal in amplitude-shaken optical lattices

Tanjun Zhou, Zhongcheng Yu, Zhihan Li, Xuzong Chen, and Xiaoji Zhou

1 State Key Laboratory of Advanced Optical Communication Systems and Networks, Department of Electronics, Peking University, Beijing 100871, China
2 School of Physics, Peking University, Beijing 100871, China
3 Collaborative Innovation Center of Extreme Optics, Shanxi University, Taiyuan, Shanxi 030006, China

(Dated: March 10, 2020)

With topological semimetal developing, semimetal with nodal-line ring comes into people’s vision as a powerful candidate for practical application of topological devices. We propose a method using ultracold atoms in two-dimensional amplitude-shaken bipartite hexagonal optical lattice to simulate nodal-line semimetal, which can be achieved in experiment by attaching one triangular optical lattice to a hexagonal optical lattice and periodically modulating the intensity and position of the triangular lattice. By amplitude shaking, a time-reversal-symmetry-unstable mode is introduced into the bipartite optical lattice, and then the nodal-line semimetal is gotten by adjusting the proportion of such mode and the trivial mode of hexagonal lattice. Through calculating the energy spectrum of effective Hamiltonian, the transformation from Dirac semimetal to nodal-line semimetal is achieved by changing shaking parameters. We also study the change of Berry curvature and Berry phase in the transformation, which provides guidance on measuring the transformation in experiment. By analyzing the symmetry of the system, the emergence of the time-reversal-symmetry-unstable mode is researched. This proposal provides a way to research the pure nodal-line semimetal without the influence of other bands, which may contribute to the study of those unique features of surface states and bulk states of nodal-line semimetal.

I. INTRODUCTION

Since Hermann Weyl found a massless solution to the Dirac equation [1] in 1929, research of Weyl fermion has attracted intensive attention. Last century, neutrino was considered as a strong candidate of Weyl fermion, until the observation of neutrino oscillation [2] shows that neutrino is not massless. Recently a new breakthrough about Weyl fermion has been achieved — a gapless semimetal characterized by topological invariant was realized in photonics, condensed matter, and cold atoms [3–7], named Weyl semimetal. In Weyl semimetal, one Dirac point separates into two Weyl points by breaking time-reversal symmetry or inversion symmetry, where two bands disperse linearly and intersect [8, 9], and low-energy excited electrons in a Weyl semimetal behave as Weyl fermion [9–11]. Through research on Weyl semimetals, a new topological semimetal has been discovered, which is called nodal-line semimetal [12].

Comparing with Weyl semimetal where the band crossing points are double degenerate, in nodal-line semimetal, however, the valence and conduction bands cross in momentum space and form a ring-shaped nodal line, which can be considered as that Dirac nodes or Weyl nodes couple into one-dimensional line or loop [13–18]. In bulk states, the unusual electromagnetic and transport response [19–22] have attracted a great deal of interest. In surface states, different from the Fermi arc surface states of Weyl semimetals, nodal-line semimetals have drumhead surface states [23, 24], which may demonstrate the presence of interactions [22]. Those unique features make nodal-line semimetal to become a strong candidate to fill in the gap between fundamental physics of topological materials and practical applications in quantum devices [25]. But, due to its complexity, the condensed matter system found with clear nodal-line ring are rare, which increases the difficulty of studying nodal-line semimetals in condensed matter physics [22–24].

On the other hand, the development of artificial gauge field have paved the way for simulating topological materials by using ultracold atoms [26–31]. Furthermore, due to high controllability, methods with ultracold atoms in optical lattice are widely used to simulate unique topological phenomenon, including the measurement of second Chern number [32], the observation of topologically protected edge states [33, 34]. As for Weyl semimetal, the chiral interaction and more topological information of band structure have been observed by using ultracold atoms in cubic optical lattice [35–37]. With the development of corresponding technologies, recently, 3D spin-orbit coupled ultracold atoms in optical lattice has been used in simulation of nodal-line semimetal [38].

In this paper, we propose a method to simulate nodal-line semimetal based on ultracold atoms in amplitude-shaken bipartite hexagonal optical lattice. By periodically changing potential well depth of the bipartite hexagonal optical lattice, a time-reversal-symmetry-unstable mode is imported into the system which breaks the inversion symmetry. As the frequency and shaking amplitude change, energy spectrum of the optical lattice transforms from Dirac semimetal to nodal-line semimetal. Then we discuss symmetry of the system which causes the transformation, and analyze the topological characteristic of the shaking optical lattice. The Berry curvature...
FIG. 1. Schematic diagram of 2D bipartite hexagonal lattice. (a) Potential well depth at lattice point A and B of bipartite hexagonal lattice are different and can be modulated periodically. $\vec{v}_j$ are lattice vectors, $\vec{u}_j$ are vectors connecting nearest-neighbour points ($j = 1, 2, 3$). $a$ is the distance between nearest neighbor points. (b) We change the amplitude shaking of potential well depth at A and B as the form of cosine function with a phase difference $\pi$, where the orange solid line and green dotted line denote point A and B, respectively. $\omega$ and $T$ denote the frequency and period of shaking, respectively. $V_0$ is potential well depth of trivial hexagonal optical lattice and $\Delta$ is the shaken amplitude of well depth. The blue dots mark five characteristic points during a shaking period and will be mentioned later in Fig 2(d).

and Berry phase are demonstrated in the transformation process, which provide a method to detect the transformation in further experiments. Combining with the advantages of ultracold atoms, it is likely to pioneer new approach to nodal-line semimetal. Furthermore, it may serve as an important basis for future studies of symmetry of nodal-line semimetal. Comparing with existing works [38], our system has three distinguishing features: (1) We used amplitude-shaken optical lattice to simulate nodal-line semimetal, which is effective and easy to implement, while great majority of previous methods use spin-orbit coupling (SOC) in optical lattice. (2) Our method can simulate a two dimensional nodal-line semimetal, while the existing works mainly focus on three dimensional system. (3) Band structure in our system takes form of semiconductor, where the conduction and valence bands touch at nodal-line ring without crossing each other, while existing works about nodal-line semimetal are semimetal form in a great measure, which means the existence of an overlap between the bottom of the conduction band and the top of the valence band. This difference directly influences the distribution of density of states, which may cause unusual electromagnetic and transport response. Here we use the common name "nodal-line semimetal" to describe our system, while the name "nodal-line semiconductor" may be more suitable in practical terms.

The remainder of this paper is organized as follows. In Sec. II, we introduce a particular model which is called amplitude-shaken bipartite hexagonal optical lattice, and propose its feasible experimental scheme. In Sec. III, we describe the calculation to get effective Hamiltonian and derive the energy dispersion of our system. The band structure during transformation process from Dirac semimetal to nodal-line semimetal is shown and explained by symmetry in Sec. IV. Then we discuss the topological properties by calculating Berry curvature and Berry phase in certain area in Sec. V and give a conclusion in Sec. VI.

II. MODEL DESCRIPTION AND FEASIBLE EXPERIMENTAL SCHEME

A. Model description

In this model, shaking of amplitude is applied to a trivial hexagonal optical lattice, as Fig 1 (a) shows. In the figure, A and B are different points which are inequivalent in hexagonal lattice structure. $t_{NN}$ and $t_{NNN}$ denote the nearest-neighbor tunneling coefficient and next-nearest-neighbor tunneling coefficient, respectively. And $v_j$ are...
lattice vectors, where \( \vec{v}_1 = (-\frac{3}{2}a, -\frac{\sqrt{3}}{2}a) \), \( \vec{v}_2 = (0, \sqrt{3}a) \) and \( \vec{v}_3 = (\frac{3}{2}a, -\frac{\sqrt{3}}{2}a) \). \( \vec{u}_j \) are vectors connecting nearest-neighbour points, where \( \vec{u}_1 = (-\frac{\sqrt{3}}{2}a, \frac{1}{2}a) \), \( \vec{u}_2 = (a, 0) \) and \( \vec{u}_3 = (-\frac{\sqrt{3}}{2}a, -\frac{1}{2}a) \). \( a = 2\frac{\sqrt{3}}{3} \lambda \) is the distance between nearest neighbor points, which is the side length of smallest hexagon, where \( \lambda \) is the wavelength of laser beams forming the hexagonal optical lattice.

The Hamiltonian \( \hat{H} \) of the system can be written as the Graphene-like first-order Hamiltonian hexagonal lattice. The Hamiltonian \( \hat{H} \) of the system can be written as the Graphene-like zeroth-order Hamiltonian hexagonal lattice. The Hamiltonian \( \hat{H} \) of the system can be written as the Graphene-like zeroth-order Hamiltonian hexagonal lattice. The Hamiltonian \( \hat{H} \) of the system can be written as the Graphene-like zeroth-order Hamiltonian hexagonal lattice.

According to single-particle two-bands tight-binding model, \( \hat{H}_0 \) can be written as:

\[
\hat{H}_0 = \sum_i V_0 c_i^\dagger c_i + \sum_{\langle i,j \rangle \text{ and } i \neq j} t_{ij} c_i^\dagger c_j
\]

where \( i \) represents each node of bipartite hexagonal lattice, and \( c_i^\dagger \) and \( c_i \) denote the creation and annihilation operator at node \( i \). \( t_{ij} \) denotes the tunneling coefficient between point \( i \) and \( j \) in Graphene-like first-order Hamiltonian. And \( \sum_{\langle i,j \rangle \text{ and } i \neq j} \) denotes summation over pairs of different points.

Next, we give the expression of \( \hat{H}_1 \) when the shaking of potential well depth of takes the following form:

\[
V_i(t) = V_0 + \chi(i) \frac{\Delta}{2} \cos(\omega t)
\]

where \( \omega \) denotes the frequency of shaking, \( \chi(i) \) at point A equals to 1, while at point B equals to -1. So \( \hat{H}_1 \) is written as:

\[
\hat{H}_1 = \sum_i \chi(i) \frac{\Delta}{2} \cos(\omega t) c_i^\dagger c_i + \sum_{\langle i,j \rangle \text{ and } i \neq j} \delta t_{ij}(t) c_i^\dagger c_j
\]

where \( \delta t_{ij}(t) \) is the change of tunneling coefficient due to amplitude shaking.

Therefore, the Hamiltonian \( \hat{H} \) of the system can be written as:

\[
\hat{H} = \sum_i V_i(t) c_i^\dagger c_i + \sum_{\langle i,j \rangle \text{ and } i \neq j} t_{ij} c_i^\dagger c_j
\]

FIG. 2. The proposed experimental scheme diagram. (a) Using three ellipitical polarization laser beams at 120° each other, the bipartite hexagonal is formed. Each laser beam is formed by combining two linearly polarized light with polarization directions in the lattice plane (\( V_{\text{in}} \)) and perpendicular to the lattice plane (\( V_{\text{out}} \)). (b) Hexagonal lattice corresponds to \( V_{\text{out}} \) and Triangular lattice corresponds to \( V_{\text{in}} \). (c) Through changing the relative phases of three lasers, two different methods of overlying hexagonal lattice and triangular lattice is formed. In situation c1, potential well depth of point B is higher than A. When the intensity of triangular reduce to 0, we move the triangular lattice instantaneously in order to let potential well depth of point A become higher than B, as is the situation in c2. (d) The change of lattice potential energy along the first Brillouin zone boundary of the system in one shaking period. ①-⑤ correspond to the five characteristic points in Fig 1(b), respectively.
where \( t_{ij}(t) = t'_{ij} + \delta t_{ij}(t) \) is the tunneling coefficient between point \( i \) and \( j \) as a function of time. In subsequent calculations, we only keep the nearest and the next-nearest tunneling coefficient.

During the shaking process, since each pair of next-nearest sites belong to the same category of points, which follow identical rule of changing in potential well depth, the difference in well depth between them is always zero. Thus we can consider the next-nearest tunneling coefficient \( t_{NN} \) as a constant. And the nearest tunneling coefficient \( t_{NN} \) equals to one constant \( t_0 \) adding one term which is proportional to potential well depth difference between point A and B (See Appendix A), so we define \( t_{NN} \) as:

\[
t_{NN} = t_0 + t_1 \cos \omega t \tag{6}
\]

where \( t_1 \) is a constant which has the dimension of energy.

**B. Feasible experimental scheme**

The above 2D amplitude shaking model can be constructed with the following experimental scheme. This scheme is easy to be expanded to 3D system by adding a laser beam perpendicular to the lattice plane [42]. As Fig 2(a) shows, we use three elliptical polarization laser beams with an enclosing angle of 120° to each other to form a bipartite optical hexagonal lattice, which has been demonstrated in recent works [40, 41]. The total potential of optical lattice is written as:

\[
V(\vec{r}) = -V_{\text{out}} \sum_{i,j} \cos \left[ \left( \vec{k}_i - \vec{k}_j \right) \cdot \vec{r} - (\theta_i - \theta_j) \right] + \frac{1}{2} V_{\text{in}} \sum_{i,j} \cos \left[ \left( \vec{k}_i - \vec{k}_j \right) \cdot \vec{r} \right] \tag{7}
\]

where \( i = 1, 2, 3 \) represent three directions of wave vectors of laser, and \( \vec{k}_1 = \frac{1}{\sqrt{3}}(\sqrt{3}\pi, -\pi), \vec{k}_2 = \frac{1}{\sqrt{3}}(-\pi, -\pi), \vec{k}_3 = \frac{1}{\sqrt{3}}(0, 2\pi) \) are three wavevectors. \( \lambda \) is wavelength of laser beam, \( V_{\text{out}} \) and \( V_{\text{in}} \) denote the components perpendicular and parallel to the lattice plane, which can be controlled respectively. And the three angles \( \theta_1, \theta_2, \theta_3 \) represent the relative phases of elliptic polarization of the laser beams.

It can be considered as a triangular optical lattice adding to a hexagonal one, where \( V_{\text{out}} \) corresponds to triangular optical lattice and \( V_{\text{in}} \) corresponds to hexagonal optical lattice, as Fig 2(b) shows. Through adjusting the phase \( \theta_i \), the position of triangular optical lattice can be modulated. At first, the position of two sets of lattice is as Fig 2(c1) shows, where \( \theta_{1,2,3} = (2\pi/3, 4\pi/3, 0) \). So, potential well depth at point A is the superposition of potential wells of two sets of optical lattice, while at point B potential well depth is the superposition of the potential well of hexagonal optical lattice and the potential barrier of triangular one. Then through modulating \( V_{\text{out}} \) in the form of cosine function, potential well depth at point A and B can change in the form of Fig 1(b). In half of the period, potential well depth at point B is always higher than A. When the intensity of triangular lattice reduces to 0, which means that potential well depth of two points equals to each other, \( \theta_{1,2,3} \) should be modulated to \( (2\pi/3, 4\pi/3, 0) \) to make potential well depth reverse instantaneously. Fig 2(c2) shows the position of triangular optical lattice at this situation. The time of reversion, in theory, can reached within several \( \mu s \), and the shaking period in our protocol is around 500 \( \mu s \). As long as the time of reversion is short enough comparing with the oscillating period, the continuity of this process remains intact.

Finally the potential energy changes as Fig 2(d) shows, where \( V_0 = 10E_r, \Delta = 0.5E_r \). The subgraphs 1 to 5 correspond to five characteristic points in Fig 1(b). At the beginning of the period, the potential well of triangular optical lattice and point A are coincident, as Fig 2(c1) shows. And then in the first half period, the position of triangular optical lattice is fixed, and the intensity of triangular optical lattice change as cosine function, as subgraph Fig 2(d1)-(d4) shows. In this situation, potential well depth at point A is lower than point B. Next, when the intensity of triangular optical lattice reduce to 0, the triangular optical lattice change to the position as Fig 2(c2). In the second half period, the potential well of triangular optical lattice and point B are coincident, and potential well depth at point A is higher than point B as subgraphs d5 shows.

**III. EFFECTIVE HAMILTONIAN AND ENERGY DISPERSION RELATION OF THE FLOQUET SYSTEM**

In order to study the nodal-line semimetal, we first calculate the band structure of the system. In the above section, we derive the Hamiltonian of the system as a function of time in Equation (5). In this section, we introduce the method to drive the effective Hamiltonian and get the band structure of the system, which can be considered as averaging the \( \hat{H} \) over time.

To start with, we act an unitary transformation on \( \hat{U} \). Define unitary operator \( \hat{U} \):

\[
\hat{U} = \exp \left( \frac{i}{\hbar} \sum_{i \neq j} \int_0^t d\tau V_i(\tau) c_i^\dagger c_j \right) \tag{8}
\]

Through this unitary transform, we get \( e \)-index form \( \hat{H}' \) (See Appendix B):

\[
\hat{H}' = U \left( H(t) - i\hbar \frac{\partial}{\partial t} \right) U^\dagger - \left( -i\hbar \frac{\partial}{\partial t} \right) = - \sum_{<i,j> \text{ and } i \neq j} t_{ij} e^{i z_{ij} \sin \omega t} c_i^\dagger c_j \tag{9}
\]

where \( z_{ij} = \frac{\Delta}{2\pi} \left[ \chi(i) - \chi(j) \right] \) is a characteristic quantity to characterize the responses of amplitude shaking at different sites.
Next, the effective Hamiltonian can be gotten by using high frequency expansion. We only keep up to first-order terms, and the effective Hamiltonian takes the form (More details see Appendix C):

\[
H_{\text{eff}} = H_{\text{eff}}^{(0)} + \frac{1}{\hbar \omega} H_{\text{eff}}^{(1)} = H_{f0} + \sum_{n=1}^{\infty} \frac{[H_n, H_{-n}]}{n \hbar \omega} \tag{10}
\]

where \(H_{f0}\) is the zeroth-order term, and \(H_n\) means the \(e^{in\omega t}\) term Fourier expansion coefficients of Hamiltonian in Equation (9). Then we get the kernel of effective Hamiltonian:

\[
H_{\text{eff}} = H_{\text{eff},0} \hat{\tau} + H_{\text{eff},x} \hat{\sigma}_x + H_{\text{eff},y} \hat{\sigma}_y + H_{\text{eff},z} \hat{\sigma}_z \tag{11}
\]

where

\[
\begin{align*}
H_{\text{eff},0} &= -2t_{NNN} \sum_{j=1}^{3} \cos(\vec{k} \cdot \vec{v}_j) + \frac{12t_0 t_1}{\Delta} J_1^2(\beta) \\
H_{\text{eff},x} &= -t_0 J_0(\beta) \sum_{j=1}^{3} \cos(\vec{k} \cdot \vec{u}_j) \\
H_{\text{eff},y} &= -t_0 J_0(\beta) \sum_{j=1}^{3} \cos(\vec{\nu} \cdot \vec{u}_j) \\
H_{\text{eff},z} &= \frac{8t_0 t_1}{\Delta} J_1^2(\beta) \sum_{j=1}^{3} \cos(\vec{\nu} \cdot \vec{v}_j)
\end{align*}
\]

\(\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\) are Pauli matrices, and \(\vec{k}\) is wave vector of atomic state function. \(J_n\) means the \(n\)th order Bessel function. We define shaking factor \(\beta\) to describe the shaking:

\[
\beta \equiv \frac{\Delta}{\hbar \omega} \tag{12}
\]

\(\beta\) is the main parameter affecting the effective Hamiltonian, since it includes shaking frequency \(\omega\) and amplitude \(\Delta\). Through solving eigenvalues of the kernel of effective Hamiltonian (Equation (11)), the energy dispersion relation \(E(\vec{k})\) of lowest two bands can be gotten:

\[
E_{\pm}(\vec{k}) = H_{\text{eff},0} \pm \sqrt{H_{\text{eff},x}^2 + H_{\text{eff},y}^2 + H_{\text{eff},z}^2} \tag{13}
\]

IV. THE TRANSFORMATION FROM DIRAC SEMIMETAL TO NODAL-LINE SEMIMETAL

The value of \(J_n(\beta)\) will change as the shaking factor, as shown in Fig 3(a), where the different value of \(J_0\) and \(J_1\) corresponding to \(\beta\). With \(J_1(\beta) = 0, H_{\text{eff},z}\) is zero, but \(H_{\text{eff},y}\) have a finite quantity. \(E_+(\vec{k})\) and \(E_-(\vec{k})\) equals to each other at six Dirac points, which performs as Dirac semimetal, as Fig 3(b1) shows. It is worth mentioning that although shaking breaks the inversion symmetry, the gap between upper and lower band is still close at Dirac point. Fig 3(b2) is the sectional view of as Fig 3(b1). In the figure, the blue line means the upper band and the red line represents the lower band, which touch the former at edge of Brillouin zone.

In another situation for \(J_0(\beta) = 0, H_{\text{eff},x}\) and \(H_{\text{eff},y}\) is zero and \(H_{\text{eff},z}\) is nonzero. \(E_+(\vec{k})\) and \(E_-(\vec{k})\) equals to each other at a ring \(k_x^2 + k_y^2 = (\frac{\pi}{a})^2\). This energy dispersion relation performs as nodal-line semimetal, as Fig 3 (c1) shows. The upper and lower band touch inside the first Brillouin zone, which differs from the case in Dirac semimetal where the touch point is at the vertices of the first Brillouin zone. The most noteworthy feature of nodal-line semimetal is that nodes of two bands are continuous and form a so-called nodal-line ring, where in our model locates at \(k_x^2 + k_y^2 = (\frac{\pi}{a})^2\). Fig 3(c2) is sectional view of Fig 3(c1). The two bands touch at the nodal-line ring, and at the edge Brillouin zone the gap...
between two bands is open.

When $\beta$ changes from $J_0(\beta) = 0$ to $J_1(\beta) = 0$, the system transforms from Dirac semimetal to nodal-line semimetal. Fig 4 shows the band structure for the other value between $J_0(\beta) = 0$ and $J_1(\beta) = 0$ corresponding to the four vertical dashed red lines and two colorful curves in Fig 3(a). When the energy spectrum gradually varies from nodal-line semimetal to Dirac semimetal, the touching ring gradually opens as the Dirac points gradually close, while the average energy of two bands decreases from $0.16E_r$ to 0, as shown in Fig 4(a)-(d). In experiment, $\beta$ can be changed continuously by fixing the amplitude of potential well depth shaking and adjusting the rotating frequency continuously to observe the transformation from Dirac semimetal to nodal-line semimetal.

In Fig 3 and Fig 4, the parameters are chosen from the experimental parameters of $^{87}\text{Rb}$ atom: $V_0 = 10.0E_r$, $t_0 = 0.1538E_r$, $t_1 = 0.0118E_r$, $t_{NN} = 7.689 \times 10^{-4}E_r$, and $\Delta = 0.50E_r$, where $E_r$ is the electronic recoil energy.

The transformation from Dirac semimetal to nodal-line semimetal can be explained by symmetry as follows. The impact of amplitude shaking is reflected in Hamiltonian, so we first study the Hamiltonian $H'$. Through Jacobi-Anger expansion (ignoring terms unrelated to $\beta$), the Hamiltonian $H'$ can be written as the following form:

$$H' = \sum_{\langle i,j \rangle \ and \ i \neq j} t_{ij} e^{i\omega t} \sin \omega t c_i^\dagger c_j$$

(14)

$$= -\sum_{\langle i,j \rangle} J_0(\beta) t_{NN} c_i^\dagger c_j$$

$$- (e^{i\omega t} + e^{-i\omega t}) \sum_{\langle j \rangle} J_1(\beta) t_{NN} c_i^\dagger c_j$$

$$- o(t_{NN} c_i^\dagger c_j)$$

Where $\sum_{\langle i,j \rangle}$ means the sum of nearest-neighbor lattice nodes, and $o(t_{NN} c_i^\dagger c_j)$ represents the higher order infinitesimal term comparing to $t_{NN} c_i^\dagger c_j$. So the system mainly is composed of two modes, the weights of which are $J_0(\beta)$ and $J_1(\beta)$.

As Fig 5 shows, the expanding term of Hamiltonian $H'$ can be divided into two parts. The first term corresponds to Mode I, which is a Graphene-like hexagonal lattice Mode. When $J_1(\beta) = 0$, only mode I exists in the system, so the system performs as ordinary Dirac semimetal. In the situation, Dirac points are closed due to the spatial inversion symmetric potential energy in Mode I.

The second term of Hamiltonian $H'$ corresponds to Mode II, which is consist of two symmetrical rotating lattices. The Mode II is the same as Mode I, both of which have time-reversal symmetry, but different from Mode I, the time inversion symmetry of Mode II is unstable. In our system, the phase difference is $\pi$, so the difference of well depth can be written as cosine function, and the amplitude of two sub-modes are equivalent to each other. If we change the phase difference, the form of well depth difference between point A and B change consequently, which cause the two sub-modes of Mode II to be asymmetric and leads to the broken of time-reversal symmetry. When $J_0(\beta) = 0$, Mode I will vanish while Mode II remains existing in the system, so its valence and conducting band touch at a ring, performing as nodal-line semimetal. When $\beta$ is between the zeros of $J_0$ to $J_1$, the system is in the superposition state of two modes.

V. BERRY CURVATURE AND BERRY PHASE

In this section, we calculate the Berry curvature and Berry phase of our optical lattice system to provide a measurable quantity in experiment during the transformation from Dirac semimetal to nodal-line semimetal.

From Equation (11), we can define $\vec{h}$ as:

$$\vec{h} = \mathcal{H}_{eff.x} \cdot \hat{e}_x + \mathcal{H}_{eff.y} \cdot \hat{e}_y + \mathcal{H}_{eff.z} \cdot \hat{e}_z$$

(15)

where $\hat{e}_x, \hat{e}_y, \hat{e}_z$ are the basis vectors at $x, y, z$ direction of momentum space. The role that $\vec{h}$ plays is similar to a magnetic field coupling with the vector of Pauli matrices ($\vec{\sigma}_x, \vec{\sigma}_y, \vec{\sigma}_z$). When there is no degeneration, it leads to the evolution of Bloch vectors of two eigenstates on the Bloch sphere, the direction of which $\pm \vec{h}$ determines two Bloch eigenstates [43]:

$$\phi_{\pm}(\vec{k}) = \mp \vec{h}$$

(16)

So when the system is at the superposition state of two modes, the Berry curvature of the lowest band can be
FIG. 5. **Two shaking modes of the system.** The result of Fourier transform of Hamiltonian $\hat{H}'$ reflects two shaking modes of the system, where Mode I is a trivial Graphene-like hexagonal lattice mode and Mode II is a nontrivial time-reversal-symmetry-unstable mode, which corresponds to nodal-line semimetal.

$$
\sum_{\langle ij \rangle} J_0(\beta) t_N N c_i^\dagger c_j
$$

FIG. 6. **The change of Berry curvature during the transformation process.** (a-d) Berry curvature in the reciprocal space in the process of the system transforming from nodal-line semimetal to Dirac semimetal. $\beta = 2.43, 2.50, 2.60, 2.90$, which is correspond to the four lines in Fig 3(a), respectively. The dashed circle denotes integral region of Berry phase, which goes around one vertex of the first Brillouin Zone.
is always zero.

Recently many experiments implemented with ultracold atoms in an optical lattice system have focused on studying the Berry curvature or other topological invariant [36, 47, 48], and some researchers among them have developed mature technology to map Berry curvature [49]. So our result of Berry curvature and Berry phase can be verified in the future experiments by existing technology.

VI. CONCLUSIONS

In summary, we propose a feasible scheme to simulate nodal-line semimetals with ultracold atoms in amplitude-shaken optical lattice. We derive the effective Hamiltonian of the Floquet system, and by calculating the band structure, the transformation from Dirac semimetal to nodal-line semimetal is observed. When the shaking factor \( \beta \), which is determined by the shaking amplitude and frequency, is at zeros of the first order Bessel function, the band structure performs as Dirac semimetal, and when shaking factor is at the zeros of the zeroth-order Bessel function, the band structure performs as nodal-line semimetal. Through Fourier transform, we divide the shaking into two modes, which explain the above transformation. The change of Berry curvature and Berry phase during the transformation process shows the topological characteristics of our system. Through changing the phase difference of the amplitude shaking at different sites, time-reversal symmetry will be broken, which furthermore causes the broken system’s time-reversal symmetry, which can help us to research new topological semimetals.

VII. ACKNOWLEDGEMENT

We thank Xiaopeng Li, Wenjun Zhang, Yuan Zhan for helpful discussion. This work is supported by the National Basic Research Program of China (Grant No. 2016YFA0301501) and the National Natural Science Foundation of China (Grants No. 61727819, No. 11934002, No. 91736208, and No. 11920101004).

Appendix A: Tunneling coefficient

We estimate the nearest-neighbor tunneling coefficient in our Floquet system, taken \(^{87}\text{Rb}\) atom for instance. For a hexagonal optical lattice with different well depth at point A and B, the overlapping integral of Wannier function helps us to calculate the nearest-neighbor tunneling coefficient \( t_{NN} \), which renders result consistent with Equation (6).

Fig 8 shows the change of nearest-neighbor tunneling coefficient as the difference of well depth \( (V_A - V_B)/V_A \) changes. As a result, the nearest-neighbor tunneling coefficient \( t_{NN} \) equals to one constant \( t_0 \) adding one term which is nearly proportional to potential well depth difference between point A and B in a large range (Correlation coefficient is 0.9995). In the process of changing potential well depth, the change of well depth at point A \( V_A \) is less than 20\%, and the difference of well depth \( (V_A - V_B)/V_A \) is about 35\%. The linearity will be better if the process happens in a smaller range. So the static process can be used to estimate our dynamic perturbation process. In our system, potential well depth difference between point A and B changes over time as cosine function, which leads to the conclusion that nearest-neighbor tunneling coefficient also changes as cosine function, so we use \( t_{NN} = t_0 + t_1 \cos(\omega t) \) to estimate it in calculation. Using fitting result, we can calculate that

\[
\begin{align*}
t_0 &= 0.1656 E_r - 0.2363 \frac{\Delta}{V_A} E_r \\
t_1 &= 0.2363 \frac{\Delta}{V_A} E_r
\end{align*}
\]

By substituting \( \Delta = 0.5 E_r \) and \( V_A = 10 E_r \), we get

\[
t_0 = 0.1538 E_r, \quad t_1 = 0.0118 E_r \quad (A1)
\]

As for next-nearest-neighbor tunneling coefficient, because potential well depth of the next neighbor point is always 0, we use a constant to replace the next neighbor tunneling coefficient

\[
t_{NNN} = 0.0050 E_r \quad (A2)
\]

In addition, according to Equation (10), the high frequency expansion requires shaking frequency \( \omega \) to be far
greater than \( H_{f0}/\hbar \). In our system, it requires that difference of potential well depth \( \Delta \) is larger than 0.15 \( V_A \), which meets the linear range.

**Appendix B: Unitary transformation of Hamiltonian**

The unitary operator \( U \) can be obtained by substituting Equation (3) into Equation (8):

\[
U(t) = \exp \left[ \frac{i}{\hbar} \sum_i \int_0^t d\tau \cdot \chi(i) \frac{\Delta}{2} \cos(\omega \tau) c_i^\dagger c_i \right]
\]

\[
= \exp \left[ \frac{i}{\hbar} \sum_i \chi(i) \frac{\Delta}{2\omega} \sin(\omega \tau) c_i^\dagger c_i \right]
\]

(\text{B1})

Then we get

\[
U \left( -i\hbar \frac{\partial}{\partial t} \right) U^\dagger = -i\hbar \frac{\partial}{\partial t} - \sum_i \frac{\Delta}{2} \cos(\omega t) \chi(i) c_i^\dagger c_i
\]

(\text{B2})

Define \( U'_k(t) \) as

\[
U'_k(t) = \exp \left[ \left( \frac{i}{\hbar} \frac{\Delta}{2\omega} \sin(\omega t) \chi(k) \right) c_k^\dagger c_k \right]
\]

(\text{B3})

According to Baker-Campbell-Hausdorff formula,

\[
e^\hat{A} \hat{B} e^{-\hat{A}} = \hat{B} + [\hat{A}, \hat{B}] + \frac{1}{2!} [\hat{A}, [\hat{A}, \hat{B}]] + \ldots
\]

(\text{B4})

We can get

\[
U(-t_{ij} c_i^\dagger c_j) U^\dagger = \sum_k U'_k(-t_{ij} c_i^\dagger c_j) \sum_k U'^\dagger_k
\]

\[
= -t_{ij} e^{\frac{i}{\hbar} \sum \frac{\Delta}{2} \sin(\omega t) [\chi(i) - \chi(j)] c_i^\dagger c_j}
\]

(\text{B5})

The transformed Hamiltonian was finally obtained

\[
H' = U \left( H(t) - i\hbar \frac{\partial}{\partial t} \right) U^\dagger - \left( -i\hbar \frac{\partial}{\partial t} \right)
\]

\[
= \sum_i V_i(t)(c_i^\dagger c_j - \sum_{\langle i,j \rangle and \ i \neq j} t_{ij} e^{iz_{ij} \sin(\omega t)} c_i^\dagger c_j
\]

\[-i\hbar \frac{\partial}{\partial t} - \sum_i \frac{\Delta}{2} \cos(\omega t) \chi(i) c_i^\dagger c_i + i\hbar \frac{\partial}{\partial t}
\]

\[-\sum_{\langle i,j \rangle and \ i \neq j} t_{ij} e^{iz_{ij} \sin(\omega t)} c_i^\dagger c_j
\]

(\text{B6})

where the first term in Equation (2) was neglected, since the zero point of energy has been set at \( V_0 \), and \( z_{ij} = \frac{\Delta}{2\omega} [\chi(i) - \chi(j)] \).

**Appendix C: Fourier expansion and derivation of effective Hamiltonian**

By a Jacobi-Anger expansion, \( e^{iz \sin \theta} = \sum_{n=-\infty}^{+\infty} J_n(z) e^{in\theta} \), we expand \( H' \) in Equation (9), taking both nearest-neighbor and next-nearest-neighbor tunneling into consideration, then

\[
H'(t) = -\sum_{n=-\infty}^{+\infty} e^{inz \omega t} \left( \sum_{\langle i,j \rangle} \left( t_{0} J_n(z_{ij}) + \frac{t_{1}}{2} \left[ J_{n-1}(z_{ij}) + J_{n+1}(z_{ij}) \right] \right) c_i^\dagger c_j
\]

\[+ \sum_{\langle\langle i,j \rangle \rangle} J_n(0) t_{NNNC} c_i^\dagger c_j \]

(\text{C1})

where \( \sum_{\langle i,j \rangle} \) denotes the summation over nearest-neighbor nodes, and \( \sum_{\langle\langle i,j \rangle \rangle} \) denotes the summation over next-nearest-neighbor nodes. Then we can obtain the Fourier expansion coefficients of Hamiltonian

\[
H_n = -\sum_{\langle i,j \rangle} \left( t_{0} + t_{1} \frac{n}{z_{ij}} \right) J_n(z_{ij}) c_i^\dagger c_j
\]

\[+ \sum_{\langle\langle i,j \rangle \rangle} J_n(0) t_{NNNC} c_i^\dagger c_j \]

(\text{C2})

From the Floquet theory, we can derive the formula to calculate effective Hamiltonian\( [50, 51] \)

\[
H_{eff} = H_{eff}^0 + \frac{1}{\hbar \omega} H_{eff}^1 = H_{0} + \sum_{n=1}^{\infty} \frac{H_n}{\hbar \omega} \]

(\text{C3})
where higher order terms have been neglected due to high frequency approximation. The calculation of substituting Equation (C2) into equation (C3) is shown below.

For $n = 0$ term,

$$H_{f0} = -\sum_{\langle ij \rangle} t_0 \mathcal{J}_0(z_{ij}) c_i^\dagger c_j - \sum_{\langle \langle ij \rangle \rangle} t_{NNN} c_i^\dagger c_j$$

$$= H_{0,1} + H_{0,2}$$

(C4)

where $H_{0,1}$ denotes the summation over nearest-neighbor nodes, and $H_{0,2}$ denotes the summation over next-nearest-neighbor nodes. For $H_{0,1}$, because $\mathcal{J}_0(z_{ij}) = \mathcal{J}_0(z_{ij})$, we can get

$$H_{0,1} = -t_0 \mathcal{J}_0(\beta) \sum_k (a_k^\dagger b_k - u_k)$$

$$+ t_{NN} c_i^\dagger c_j + u_i + u_j + h.c.$$  

(C5)

where $\beta \equiv \frac{2\pi}{\lambda}$, $a_i$, $b_j$ denote the annihilation operators of lattice site $A_i$, $B_j$. The first term describes the tunneling from $B_j$ to $A_i$, while the second term is the Hermitian conjugate of former one, describes the tunneling from $A_i$ to $B_j$. The $\vec{r}_i$ is the lattice vector for bipartite hexagonal lattice, and the $u_i$ is nearest-neighbor vector.

Considering the creation and annihilation operators as periodic functions in real space, we can make use of the Fourier transformation to get the corresponding creation and annihilation operators in momentum space. For $n > 0$ terms,

$$H_n = -\sum_{\langle ij \rangle} \left( t_0 \mathcal{J}_n(z_{ij}) + \frac{t_1}{2} \left[ \mathcal{J}_{n-1}(z_{ij}) + \mathcal{J}_{n+1}(z_{ij}) \right] \right) c_i^\dagger c_j$$

(C8)

According to Equation (C3),

$$H_{eff}^{(1)} = \sum_{n=1}^{\infty} \frac{[H_n, H_{-n}]}{n}$$

$$= \frac{4t_0t_1}{\beta} \mathcal{J}_1(\beta)^2$$

$$\times \left\{ 3 \sum_i [a_i^\dagger b_i^\dagger + \sum_{\langle \langle ij \rangle \rangle} [a_i^\dagger a_j - b_i^\dagger b_j] \right\}$$

$$= \sum_k (a_k^\dagger b_k) \left( H_{11} + H_{12} \right) \frac{\mathcal{J}_1(\beta)^2}{\beta}$$

$$\times \sum_{j=1}^{\langle\rangle} \cos(\vec{k} \cdot \vec{v}_j)$$

which uses the commutation relationship $[c_i^\dagger c_i, c_j^\dagger c_j] = \delta_{ij} c_j^\dagger c_j - \delta_{j0} c_j^\dagger c_j$. And $H_{11} = 12t_0t_1 \frac{\mathcal{J}_1(\beta)^2}{\beta}$, $H_{12} = 8t_0t_1 \frac{\mathcal{J}_1(\beta)^2}{\beta}$ $3 \sum_{j=1}^{\langle\rangle} \cos(\vec{k} \cdot \vec{v}_j)$.

Combining the results of Equation (C6), (C7) and (C9), we can draw the conclusion that

$$H_{eff} = H_{eff}^{(0)} + \frac{1}{\hbar \omega} H_{eff}^{(1)}$$

$$= \sum_k (a_k^\dagger b_k) \left( \mathcal{H}_{eff,11}(\vec{k}) + \mathcal{H}_{eff,22}(\vec{k}) \right) \left( \begin{array}{c} a_k \\ b_k \end{array} \right)$$

(C10)

where

$$\mathcal{H}_{eff,11} = \left[ -2t_{NNN} + \frac{8t_0t_1 \mathcal{J}_1(\beta)^2}{\hbar \omega} \right] \sum_{j=1}^{\langle\rangle} \cos(\vec{k} \cdot \vec{v}_j)$$

$$+ \frac{12t_0t_1 \mathcal{J}_1(\beta)^2}{\hbar \omega} \sum_{j=1}^{\langle\rangle} \cos(\vec{k} \cdot \vec{v}_j)$$

(C11)

$$\mathcal{H}_{eff,22} = \left[ -2t_{NNN} - \frac{8t_0t_1 \mathcal{J}_1(\beta)^2}{\hbar \omega} \right] \sum_{j=1}^{\langle\rangle} \cos(\vec{k} \cdot \vec{v}_j)$$

$$+ \frac{12t_0t_1 \mathcal{J}_1(\beta)^2}{\hbar \omega} \sum_{j=1}^{\langle\rangle} \cos(\vec{k} \cdot \vec{v}_j)$$

(C12)

and

$$\mathcal{H}_{eff,12} = \mathcal{H}_{eff,21}^* = -t_0 \mathcal{J}_0(\beta) \sum_{j=1}^{\langle\rangle} e^{-i\vec{k} \cdot \vec{v}_j}$$

(C13)

The $2 \times 2$ matrix in the above equation is the so-called kernel of Hamiltonian, denoted as $\mathcal{H}_{eff}$, which can be spanned by 2-ranked identity matrix and three 2D Pauli matrices according to linear algebraic theory. The final result is exactly Equation (11) in the article.
