Effect of incommensurate potential on nodal-link semimetals

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We explore the effect of an incommensurate potential on nodal-link semimetals. For system with surface states, we show the nodal-link semimetal undergoes a series of phase transitions: first into a metallic phase, then to a loop semimetal phase and back to a metallic phase with increasing the strength of incommensurate potential. The phase transitions are unveiled by analyzing the properties of energy spectra and wave functions. We also study the system without surface states and find that the Fermi surface evolves from lines to loops before the system enters into a metallic phase when increasing the incommensurate potential strength.

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I. INTRODUCTION

The recent discoveries of topological phases of matters, which contain both gapped systems and gapless semimetals12, have vastly deepened our understanding of quantum phases of matter. The gapped topological states, including topological insulators and topological superconductors34, can be well described by the underlying symmetries5–7 and associated topological invariants. While for the gapless semimetals, the crossings of the conduction and valance band may occur at some discrete points in Brillouin zone (BZ), such as Weyl and Dirac semimetal7,19, or along some closed loops, corresponding to topological nodal line semimetals20–24. There exist some possible configurations for two nodal loops. They can be isolated, touched at one point, or linked with each other, known as nodal link semimetals22,25. The nontrivial linking of the nodal lines is described by a Hopf link number and may bring exotic topological properties to the system. A model Hamiltonian for Hopf insulators in a solid-state quantum simulator has been implemented and the experimental observation of their topological properties was also reported26.

The effect of disorder on topological state is an important question, especially for topological semimetals, due to the lack of protection of a finite energy gap and vanishing density of states (DOS) at the Fermi level. For Dirac27,30 and Weyl21,28 semimetals, its have been found that the semimetal phases are robust against weak disorder and generally the system would first enter into a metal phase before becoming an insulator by increasing the strength of disorder. The effect of an incommensurate potential on the Weyl semimetals was firstly studied in Ref.39 by adding a quasiperiodic potential along one direction of the lattice, which unveils a transition from a Weyl semimetal to a metal driven by the incommensurate potential. For three-dimensional incommensurate potentials, it has been demonstrated recently by Pixley et al.40 that there exist Weyl semimetal (WSM)-metal-semimetal-metal phase transitions by increasing the incommensurate potential strength. The incommensurate potential is quasiperiodic, lying between a random potential and periodic potential and has been widely used in cold atom experiment41. It can induce many interesting phenomenon, such as ballistic transport42 and finite localized-delocalized transition in one dimension43,44 distinct from the random potential.

Taking advantages of these features, a natural and interesting question is then what is the fate of the nodal-link semimetal by applying such an incommensurate potential? To answer this question, we consider the simplest case with incommensurate potential applied only in one spatial direction. The introduced incommensurate potential only destroys the translation invariance in one dimension, whereas momentums in other two direction are still good quantum numbers. Such a choice not only simplifies our calculation and overcomes the size difficulty, but also provides important insights29,30 towards the disorder effects of nodal-link semimetals under different boundary conditions.

This paper is organized as follows: in Sec. II we introduce the three dimensional Hamiltonian with nodal-link Fermi surface in the presence of a one dimensional incommensurate potential. We then consider two different cases depending on the existence of surface states and analysis the phase transitions by increasing the strength of incommensurate potential. A brief summary is given in Sec. III.

II. MODEL AND RESULTS

A general two-band Bloch Hamiltonian can be written as:

$$H_0(k) = d_0(k)| + d_1(k)\tau_x + d_2(k)\tau_y + d_3(k)\tau_z,$$

where $k = (k_x, k_y, k_z)$ and $\tau_i$ ($i = x, y, z$) is Pauli matrix. For a spinless system, the time reversal operator $T$ and spatial inversion operator $P$ act on the Hamiltonian through $TH(k)T^{-1} = H^\ast(-k)$ and $PH(k)P^{-1} = H^\ast(-k)$, respectively. We assume the $H(k)$ satisfy the $PT$ symmetry36, $PTH(k)(PT)^{-1} = H^\ast(k)$, which requires that $d_3(k) = 0$. We further set $d_0(k) = 0$ without loss of generality. As a frequently-used example, we
Fermi surface contains two linked rings as shown in Fig. 1(a). We consider the half-filling case and the zero energy Fermi surface states. When the incommensurate potential is added, the Fermi surface shrinks to lines on the surface BZ as shown in Fig. 2(g) and the inset is that $\rho(0)$ as a function of $V$ for $L = 300$ and $L = 600$.

\[ d_x = 2 \sin k_x \sin k_z + 2 \sin k_y (m_0 - \sum_{i=x,y,z} \cos k_i), \]

\[ d_z = \sin^2 k_x + \sin^2 k_y - \sin^2 k_z - (m_0 - \sum_{i=x,y,z} \cos k_i)^2. \]  

We consider the half-filling case and the zero energy Fermi surface is determined by $d_x = d_z = 0$. For $1 < m_0 < 3$, the Fermi surface contains two linked rings as shown in Fig. 1(a) with $m_0 = 2.5$, whereas it contains two unlinked rings when $m_0 > 3$ as shown in Fig. 1(b) with $m_0 = 3.2$. One of the rings satisfies $k_x = k_y$ and $\sin k_z = m_0 - \sum_{i=x,y,z} \cos k_i$, the other satisfies $k_x = -k_y$ and $\sin k_z = \sum_{i=x,y,z} \cos k_i - m_0$. If we take periodic boundary conditions (PBC) along the $x$ and $y$ directions and open boundary conditions (OBC) in the $z$ direction, $k_z$ will no longer be a good quantum number. In Fig. 2(a), we show the energy spectra as a function of $k_x$ by fixing $k_y = 0$, where the $L_x \times L_y \times L_z$ cubic lattice is set as $L_x = L_y = 100a$ and $L_z = La$. For convenience, we set the lattice constant $a = 1$ and $m_0 = 2.5$ in the following context. We can clearly observe the emergence of surface states connecting the projected nodal points. The corresponding zero energy surface flat bands localized at $z = 0$ and $\pi = L_z = La$ are shown in the blue area of Fig. 2(f).

We then add an incommensurate potential along the $z$ direction. The Hamiltonian becomes

\[ H = H_0 + V \sum_{j,l} \cos(2\pi\alpha l)n_{i,j,l}, \]  

where $n_{i,j,l} = a_{i,j,l}^\dagger a_{i,j,l}$ and $\alpha$ is an irrational number, which is chosen as $\alpha = (\sqrt{5} - 1)/2$ without loss of generality. For fixed $k_x$ and $k_y$, the Hamiltonian (3) can be written in real space by using Fourier transformation:

\[ a_{k_x,k_y,0}^\dagger = \frac{1}{\sqrt{L_x L_y}} \sum_{\ell} e^{i(2\pi\alpha \ell)k_y} a_{\ell,k_y,0}^\dagger, \]

where $\gamma = A, B$ label the inequivalent sublattice of the $2 \times 2$ matrix. $a_{k_x,k_y,0}^\dagger$ ($a_{k_x,k_y,0}$) is the annihilation (creation) operator on the sublattice $A$ ($B$) of the $l-th$ layer along the $z$ direction. The $n$-th eigenstate of the Hamiltonian (3) can be generally represented as $|\Psi_n\rangle = \sum_{j,l} \psi_{n,i,j,l}^A |\psi_{n,i,j,l}^B\rangle$. Then the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$ can be reduced to the following form

\[ E_{n,k_x,k_y} |\psi_{n,j,B}\rangle = (m_0 - \cos k_x - \cos k_y)\psi_{n,j-1,B} + (i \sin k_x - \sin k_y)\psi_{n,j+1,B} - (i \sin k_x + \sin k_y)\psi_{n,j-1,B} + \sin^2 k_x + \sin^2 k_y - (m_0 - \cos k_x - \cos k_y)^2 + 1 + V \cos(\pi\alpha j)|\psi_{n,j,B}\rangle + 2 \sin k_x (m_0 - \cos k_x - \cos k_y)\psi_{n,j,B}. \]

Here $j$ is the $j-th$ layer along the $z$ direction of the system and $E_{n,k_x,k_y}$ is the $n$-th eigenvalue of the Hamiltonian at $(k_x, k_y)$, which can be easily solved by diagonalizing the $2L \times 2L$ Hamiltonian matrix.

To see how the nodal-link semimetals are changed with the increasing of incommensurate potential strength, we introduce the DOS defined as

\[ \rho(E) = \frac{1}{2L_x L_y L_z} \sum_{i=1}^{2L_x-1} \sum_{j=1}^{2L_y-1} \sum_{\ell=1}^{2L_z-1} \delta(E - E_{i,j,\ell}). \]  

where $k_x = \frac{2\pi}{L_x} i_x$ and $k_y = \frac{2\pi}{L_y} i_y$ are the quantized momenta along periodic directions. Numerically, the $\delta$ function in Eq. (5) can be approximated by using a Gaussian function. For $\sigma \approx 0.01$ in the subsequent calculations.

The zero energy DOS $\rho(0)$ with respect to the strength of incommensurate potential $V$ is shown in Fig. 3(c). Without the incommensurate potential, $V = 0$, the zero energy DOS takes a finite value, consistent with the existence of middle surface states. When the incommensurate potential is added, these surface states bend downward to $E < 0$, as shown in Fig. 3(b), where we show the energy spectra as a function of $k_x$ for fixed $k_y = 0$ and $V = 1$. The $E = 0$ Fermi surface shrinks to lines on the surface BZ as shown in Fig. 3(g) and $\rho(0)$ drops sharply as shown in Fig. 3(c). By further increasing $V$, for instance, $V = 1.5$, as shown in Fig. 3(c), one can find that the touched segment of the upper and lower bands near $k_x = k_y = 0$ is no longer point. Fig. 3(b) corresponds to the
is a loop semimetal phase. Further increasing the strength of the two dimensional (2D) BZ as shown in Fig. 2(i), i.e., the incommensurate potential to a finite value in the thermodynamical limit for this system with (f) $V = 0$, (g) $V = 1$, (h) $V = 1.5$, (i) $V = 4$ and (j) $V = 6$. Here $L = 300$.

FIG. 2. (Color online) The energy spectra as a function of $k_x$ under OBC along z direction for fixed $k_y = 0$ with the incommensurate potential strength (a) $V = 0$, (b) $V = 1$, (c) $V = 1.5$, (d) $V = 4$ and (e) $V = 6$. The corresponding cross section of energy dispersion $E(k_x, k_y)$ at $E = 0 \pm 0.03$ (with considering the finite size effect) for this system with (f) $V = 0$, (g) $V = 1$, (h) $V = 1.5$, (i) $V = 4$ and (j) $V = 6$. Here $L = 300$.

FIG. 3. (Color online) (a) $\Delta E$ versus $1/L$ for $V = 1$ and $V = 1.5$ respectively. (b) $\Delta E_{\text{max}}$ as a function of $1/L$ for fixed $V = 4$.

cross section of energy dispersion $E(k_x, k_y)$ at $E = 0 \pm 0.03$ (with considering the size effect) with $V = 1.5$ and we see that the two-band touched segment is no longer composed of lines and there exist a surface for $E = 0$. As a result, $\rho(0)$ is a finite value in the thermodynamical limit for this case. This can also be revealed in Fig. 1(c), where no obvious difference happen for the zero-energy DOS $\rho(0)$ with different system length when $1.5 < V < 1.8$.

If the incommensurate potential strength $V$ continues to increase to $V > 1.8$, though the cross segment near $k_y = 0$ would open an energy gap, there emerges two gap closing point at finite $k_x$ as shown in Fig. 2(d) with $V = 4$. The $\rho(0)$ will drop to zero again as shown in Fig. 1(c) and the cross segment of the upper and lower bands now becomes a loop in the two dimensional (2D) BZ as shown in Fig. 2(i), i.e., this is a loop semimetal phase. Further increasing the strength of the incommensurate potential to $V > 4.6$, the upper and lower bands will touch again as shown in Fig. 2(e) with $V = 6$. The touched segment becomes a 2D region in the BZ as shown in Fig. 2(j). The corresponding $\rho(0)$ becomes a finite value as shown in Fig. 1(c) and this system enters into the metallic phase again.

To solidate the above discussions, we analyze the corresponding energy gaps. For fixed $k_x$ and $k_y$, we can define the energy gap of the upper band and the lower band near $E = 0$ as $\Delta E_{k_x, k_y} = E_{L+2, k_x, k_y} - E_{L, k_x, k_y}$, where $E_{L, k_x, k_y}$ and $E_{L+2, k_x, k_y}$ are the $L$-th and $(L + 2)$-th eigenvalues at $(k_x, k_y)$ and the eigenvalues are in ascending order. Note that we use the $(L + 2)$-th instead of $(L + 1)$-th state because at some specific $(k_x, k_y)$ the latter may correspond to the surface state, which bend downwards to $E < 0$ by increasing the incommensurate potential strength. We take a small region near $k_x = 0, k_y = 0$, e.g., $|k_x| \leq 0.01\pi, |k_y| \leq 0.01\pi$ and divide this region into $N \times N$ equal parts. Then the mean energy gap is

$$\overline{\Delta E} = \frac{1}{N^2} \sum_{k_x, k_y} \Delta E_{k_x, k_y},$$

with the summation over all the $k_x$ and $k_y$ in the chosen small region. If $\overline{\Delta E}$ approaches zero in the thermodynamical limit, the size of the zero energy Fermi surface is then bigger than this region, while if $\overline{\Delta E}$ approaches a finite value in the thermodynamical limit, the size of the Fermi surface is smaller than the chosen region. We divide the region $|k_x| \leq 0.01\pi, |k_y| \leq 0.01\pi$ into $40 \times 40$ equal parts and show $\overline{\Delta E}$ as a function of $1/L$ in Fig. 3(a). It is obvious the mean energy gap $\overline{\Delta E}$ tends to zero when $L \to \infty$ for $V = 1.5$, which means the size of the Fermi surface is bigger than $0.02\pi \times 0.02\pi$ and this system enters into a metallic phase. As a comparison, we also
show the mean energy gap $\Delta E$ for $V = 1$. It tends to a finite value when $L \to \infty$. We can further narrow this region almost to zero. In the whole process, $\Delta E$ would not tend to zero when $L \to \infty$. However, $\Delta E$ tends to zero in the thermodynamical limit when only considering the states at $k_x = 0, k_y = 0$ for $V = 1$, indicating that the system is a semimetal phase. For $V \approx 1.8 \sim 4.6$ case, the zero-energy DOS $\rho(0)$ tends to zero. In Fig. 3(b), we plot the minimum gap $\Delta E_{\text{min}} = \min(\Delta E_{k_x,k_y})$ with respect to $1/L$ for fixed $V = 4$. It tends to zero in thermodynamical limit, indicating that the energy gap would not open along the nodal loop. The system is in a loop semimetal phase.

The incommensurate potential of the $z$ direction can give rise to the extended-localization transition in this direction. To characterize it, we introduce the IPR\textsuperscript{54,55} of the system at fixed $k_x$ and $k_y$. For a normalized wave function $\psi_n$, the IPR is defined as $\text{IPR} = \sum_j (\psi^2_{n,j,A} + \psi^2_{n,j,B})^2$. The IPR approaches to zero or a finite value of $O(1)$ in the thermodynamical limit corresponding to an extended or localized state. For the filled lower band, we can further define the mean IPR\textsuperscript{56,57} as

$$\text{MIPR} = \frac{1}{L} \sum_{l=1}^{L} \sum_{j=1}^{J} (\psi^2_{n,l,A} + \psi^2_{n,l,B})^2, \quad (7)$$

which is the average of the IPRs over all the eigenstates of the lower band. Our results are summarized in Fig. 4.

In Fig. 4(a) and (c), we present the MIPR as a function of $k_x$ and $V$ with fixed $k_y = 0$ and $k_y = \pi$ respectively. In Fig. 4(b) and (d), we present the MIPR as a function of $k_y$ and $V$ by fixing $k_x = 0$ and $k_x = \pi$ respectively. From these figures, we see that there exists an extended-localization transition when increasing the incommensurate potential strength. The states around $(k_x, k_y) = (0, \pm \pi)$ are harder to be localized than those at other $k_x$ and $k_y$, while localization for the states around $(k_x, k_y) = (0, 0)$ are much easier. In Fig. 4(e), we show the MIPR as a function of $k_x$ and $k_y$ with fixed $V = 1.5$. It is clear that the states become localized in regions $k_x \in [-0.3\pi, 0.3\pi]$ and $k_y \in [-0.15\pi, 0.15\pi]$, much bigger than the size of the Fermi surface. In fact, the system can be viewed as a two-dimensional metal for $V \approx 1.5 \sim 1.8$.

In the same way, we can analyze the metallic phase for $V > 4.6$. As an example, we show the MIPR as a function of $k_x$ and $k_y$ for fixed $V = 6$ in Fig. 4(f). As compared to Fig. 4(j), the localized region completely contains the band cross section. Thus the system is a two-dimensional metal in this region.

Similar results can be obtained for systems with OBC in the $y$ direction and PBC in the $x$ and $z$ directions. However if we take OBC in the $x$ direction and PBC in the $y$ and $z$ directions, things would be different. In this case, $k_x$ and $k_y$ are good quantum numbers. A crucial difference is that there exist no edge states on the surface BZ spanned by $(k_x, k_y)$ at $V = 0$. The energy spectra as a function of $k_x$ for fixed $k_y = 0$ with different incommensurate potential strengths are shown in Fig. 5(a) $V = 0$, (b) $V = 1$, (c) $V = 2$, (d) $V = 3$ and (e) $V = 4$. Correspondingly, we also demonstrate the cross sections of energy dispersion $E(k_x, k_y)$ at $E = 0 \pm 0.03$ in Figs. 5(f)-(j).

In the absence of incommensurate potential, $V = 0$, the cross section of energy dispersion $E(k_x, k_y)$ at $E = 0 \pm 0.03$ is two lines with no surface states as shown in Fig. 5(a) and (f). By increasing $V$, one line is broken into two with unchanged end points as shown in Fig. 5(b) and (g). Further increasing $V$, e.g., $V = 2$ as shown in Fig. 5(c) and (h), the Fermi surface becomes two loops with an touching point at $k_x = 0, k_y = 0$. Keep increasing the incommensurate potential strength, e.g., $V = 3$ as shown in Fig. 5(d) and (i), this system enters into a metallic phase with the emergence of middle Fermi surface. Further increasing $V$, e.g., $V = 4$ as shown in Fig. 5(e) and (j), the two loops would merge into one loop, separated from the middle surface.

**III. SUMMARY**

In summary, we have investigated the effect of one-dimensional incommensurate potential on the nodal-link semimetals. When the potential is added along $z$ ($y$) direction, there exist surface states on the 2D surface BZ. The system undergoes several phase transition by increasing the strength of incommensurate potential: first from a nodal-link semimetallic phase to a metallic phase, then to a loop semimetal phase.
FIG. 5. (Color online) The energy spectra as a function of $k_x$ under OBC along $x$ direction for fixed $k_z = 0$ with the incommensurate potential strength (a) $V = 0$, (b) $V = 1$, (c) $V = 2$, (d) $V = 3$ and (e) $V = 4$. The corresponding cross section of energy dispersion $E(k_x, k_y)$ at $E = 0 \pm 0.03$ for this system with (f) $V = 0$, (g) $V = 1$, (h) $V = 2$, (i) $V = 3$ and (j) $V = 4$. Here $L = 300$.

and a metallic phase again. When the potential is added along $x$ direction and no surface states exist on the 2D surface BZ, the system will form two loops from the initially two Fermi lines and then the two loops merge into one closed loop. In this process, the middle closed point would not open and the system enter directly into a metallic phase.

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Appendix A

In this appendix, we give some details of derivation of Eq. (4) from Eqs. (1), (2) and (3). Since $k_x$ and $k_y$ are good quantum numbers, we take the Fourier transform: $a_{k_x,k_y,l}^\gamma = \frac{1}{\sqrt{\Gamma}} \sum_k e^{i(k_{\xi}\gamma)} a_{k_x,k_y,l}^\gamma$, where $\gamma = A, B$ and $a$ is the lattice constant. After the Fourier transform, we rewrite the Eq. (3) as:

$$H = \sum_{k_x,k_y} H(k_x,k_y),$$

with

$$H(k_x,k_y) = \sum_l \left[ 2 \sin k_y (m_0 - \cos k_x - \cos k_y) a_{k_x,k_y,l}^A \right. \\
+ (m_0 - \cos k_x - \cos k_y) a_{k_x,k_y,l+1}^A a_{k_x,k_y,l}^A \\
+ (m_0 - \cos k_x - \cos k_y) a_{k_x,k_y,l-1}^A a_{k_x,k_y,l}^A \\
+ (m_0 - \cos k_x - \cos k_y) a_{k_x,k_y,l}^A a_{k_x,k_y,l+1}^A \\
+ (m_0 - \cos k_x - \cos k_y) a_{k_x,k_y,l}^A a_{k_x,k_y,l-1}^A \\
+ \left. \sum_{l=1}^{\infty} 2 \sin k_x (m_0 - \cos k_x - \cos k_y) a_{k_x,k_y,l}^B a_{k_x,k_y,l}^B \\
+ (\sin k_x - \sin k_y) a_{k_x,k_y,l}^A a_{k_x,k_y,l+1}^A + (\sin k_y - \sin k_x) a_{k_x,k_y,l-1}^A a_{k_x,k_y,l}^A \\
\right]$$

where $a_{k_x,k_y,l}^A$ and $a_{k_x,k_y,l}^B$ ($a_{k_x,k_y,l}^A$ and $a_{k_x,k_y,l}^B$) are the annihilation (creation) operators on the sublattice A and B of the $l-$th layer along the $z$ direction for fixed $k_x$ and $k_y$, $a_{k_x,k_y,l}^A = a_{k_x,k_y,l}^A a_{k_x,k_y,l}^A$ and $n_{k_x,k_y,l}^B = a_{k_x,k_y,l}^B a_{k_x,k_y,l}^B$. The $n-$th eigenstate $|\Psi_n\rangle$ of
which are the Eqs. (4). In a similar way, we can obtain the eigenvalue equation for the case of taking OBC along $x$ or $y$ direction.

After introducing a vector $\Psi = (\psi_{n,1A}, \psi_{n,1B}, \psi_{n,2A}, \psi_{n,2B}, \ldots, \psi_{n,L-1A}, \psi_{n,L-1B}, \psi_{n,L,A}, \psi_{n,L,B})$, Eqs. (A2) can be written as a $2L \times 2L$ matrix:

$$H(k_x, k_y) = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

where

$$A_{ij} = \begin{pmatrix} A_{ij} & B_{ij} \\ A_{ij} & B_{ij} \end{pmatrix}$$

with $A_{11} = \sin^2 k_x + \sin^2 k_y - (m_0 - \cos k_x - \cos k_y)^2 - 1 + V \cos(2\alpha j)$, $A_{12} = 2 \sin k_x(m_0 - \cos k_x - \cos k_y)$, $A_{21} = 2 \sin k_x(m_0 - \cos k_x - \cos k_y)$ and $A_{22} = -\sin^2 k_x - \sin^2 k_y + (m_0 - \cos k_x - \cos k_y)^2 + 1 + V \cos(2\alpha j)$, and

$$B = \begin{pmatrix} m_0 - \cos k_x - \cos k_y & i \sin k_x - \sin k_y \\ i \sin k_x - \sin k_y & -m_0 + \cos k_x + \cos k_y \end{pmatrix}.$$
