ISSN 1674-1056
http://cpb.iphy.ac.cn
http://iopscience.iop.org/cpb
中国物理 B
Chinese Physics
中国物理 Chinese Physics B

Quantum critical duality in two-dimensional Dirac semimetals

Jiang Zhou(周江), Ya-Jie Wu(吴亚杰), Su-Peng Kou(寇谡鹏)

Citation: Chin. Phys. B . 2019, 28(1): 017402. **doi:** 10.1088/1674-1056/28/1/017402
Journal homepage: http://cpb.iphy.ac.cn; http://iopscience.iop.org/cpb

What follows is a list of articles you may be interested in

Macroscopic resonant tunneling in an rf-SQUID flux qubit under a single-cycle sinusoidal driving

Jianxin Shi(史建新), Weiwei Xu(许伟伟), Guozhu Sun(孙国柱), Jian Chen(陈健), Lin Kang(康琳), Peiheng Wu(吴培亨)

Chin. Phys. B . 2017, 26(4): 047402. **doi:** 10.1088/1674-1056/26/4/047402

Quantum critical behavior in an antiferromagnetic heavy-fermion Kondo lattice system $(Ce_{1-x}La_x)_2Ir_3Ge_5$

Rajwali Khan, Qianhui Mao(毛乾辉), Hangdong Wang(王杭栋), Jinhu Yang(杨金虎), Jianhua Du(杜建华), Binjie Xu(许彬杰), Yuxing Zhou(周宇星), Yannan Zhang(张燕楠), Bing Chen(陈斌), Minghu Fang(方明虎)

Chin. Phys. B . 2017, 26(1): 017401. **doi:** 10.1088/1674-1056/26/1/017401

Thermodynamics around magnetic phase transitions in alternating double-chain spin systems

Ding Lin-Jie, Zhong Yuan, Fan Shuai-Wei, Zhu Li-Ya

Chin. Phys. B . 2014, 23(12): 127401. **doi:** 10.1088/1674-1056/23/12/127401

Perforated nanocap array: Facile fabrication process and efficient surface enhanced Raman scattering with fluorescence suppression

Wang Jun, Huang Li-Qing, Tong Hui-Min, Zhai Li-Peng, Yuan Lin, Zhao Li-Hua, Zhang Wei-Wei, Shan Dong-Zhi, Hao Ai-Wen, Feng Xue-Hong

Chin. Phys. B . 2013, 22(4): 047301. **doi:** 10.1088/1674-1056/22/4/047301

Quantum critical duality in two-dimensional Dirac semimetals*

Jiang Zhou(周江)[1], Ya-Jie Wu(吴亚杰)[2], and Su-Peng Kou(寇谡鹏)[3,†]

[1] Department of Physics, Guizhou University, Guiyang 550025, China
[2] School of Science, Xi'an Technological University, Xi'an 710032, China
[3] Department of Physics, Beijing Normal University, Beijing 100875, China

(Received 20 June 2018; revised manuscript received 27 October 2018; published online 12 December 2018)

Quantum criticality is closely related to the existence of two phases with unrelated symmetry breaking. In this paper, we study Néel and Kekulé valence bond state (VBS) quantum criticality in Dirac semimetals with four-fermion interactions. Our results show that all possible dynamical masses yield the same critical coupling, which exhibits the phenomenon that all possible phases meet at a multicritical point (e.g., a tricritical point for the Néel, Kekulé-VBS and semimetallic phases). In terms of the well-established Wess–Zumino–Witten field theory, we investigate the typical criticality for the transition between Néel and Kekulé-VBS phases, and the compatible Néel–Kekulé-VBS mass matrices imply the existence of a non-Landau transition between the Néel and Kekulé-VBS phases. We show the existence of mutual duality in the defect-driven Néel–Kekulé-VBS transition near the non-Landau critical point and find that this mutual duality results from the presence of a mutual Chern–Simons term. We also study the mutual duality based on dual topological excitations.

Keywords: quantum criticality, duality, semimetal–insulator transition, spin–charge separation

PACS: 74.40.Kb, 73.22.Gk, 71.30.+h **DOI:** 10.1088/1674-1056/28/1/017402

1. Introduction

The study of quantum phases of matter and phase transitions in strongly correlated systems is one of the central issues of modern condensed matter physics.[1,2] Owing to strong interaction effects, interacting electrons on a two-dimensional lattice exhibit rich Mott physics and lead to many novel phenomena involving quantum phases. Recently, in the context of two- and three-dimensional semimetals, a fermion–boson mixed system has been proposed to describe a Landau-forbidden quantum phase transition that gives rise to fermion-induced quantum critical points (FIQCPs)[3–6] and a fluctuation-induced continuous phase transition with hidden degrees of freedom.[7–9] An FIQCP is an example of a type II Landau-forbidden transition, whereas an example of a type I Landau-forbidden transition is provided by the deconfined quantum critical point (QCP) in a quantum magnet.[10]

Graphene is a two-dimensional Dirac semimetal phase, with its low-energy excitations exhibiting $(2+1)$-dimensional massless Dirac fermions. Based on the graphene structure, various insulating phases can be induced at the level of the fermionic spectrum, and these are relevant to a variety of interesting phenomena, including the quantum spin Hall effect,[11,12] the quantum anomalous Hall effect,[13,14] topological node-line semimetallic behavior,[15,16] topological superconductivity,[17] and metal–insulator transitions.[18–20] Over the past decade, the Mott physics of interacting electrons in two spatial dimensions has been investigated extensively.[19–26] Recent theoretical and numerical studies have shown that the semimetal–insulator transition with electron correlation and emergent fluctuations (i.e., gauge fields or strong fermion fluctuations) exhibits an exotic continuous phase transition and a non-Landau–Ginzburg–Wilson transition[6,7,27–29] and that the transition of a gapless fermion to an order parameter with emergent symmetry should become a second-order transition.[3,7,29] The fluctuations of emergent degrees of freedom give rise to rich quantum criticality behavior, and the various QCPs associated with this behavior have been shown to belong to the Gross–Neveu–Yukawa (GNY) universality class.[30–32] Meanwhile, recent large-scale quantum Monte Carlo simulations have confirmed that the quantum criticality in interacting Dirac semimetals belongs to a special Gross–Neveu universality class.[23,33,34] Thus, the $(2+1)$-dimensional GNY theory is closely related to the dynamical mass generation, and thus to the metal–insulator transition in correlated fermion systems.[35]

In this paper, we introduce general GNY interactions, and study typical Néel–Kekulé valence band state (VBS) quantum criticality in Dirac semimetals in order to understand the non-Landau continuous transition. This idea is motivated by the classification of mass in two-dimensional electronic systems.[36] We find that the general GNY interaction gives rise to a critical four-fermion coupling, beyond which the broken microscopic symmetry yields a general mass term for fermions. The induced mass term corresponds to modulation of a special fermion bilinear and is related to the presence of an insulating phase. Theories with compatible or-

*Project supported by the National Natural Science Foundation of China (Grant Nos. 11647111, 11504285, and 11674026) and the Research Start-up Funds of Guizhou University, China (Grant No. 201538).

†Corresponding author. E-mail: spkou@bnu.edu.cn

© 2019 Chinese Physical Society and IOP Publishing Ltd

ders have been suggested for describing continuous quantum criticality,[36–39] for example, the compatible Néel VBS orders of a deconfined quantum critical point.[10,40] Within a similar formalism, we show that the Yukawa-type coupling between the Néel–Kekulé-VBS order and the fermion fields will lead to a pure bosonic action. The emergence of two symmetry-unrelated orders in the vicinity of the critical transition (i.e., Néel and Kekulé-VBS) reveals the non-Landau quantum criticality, and the low-energy theory for the fluctuating Néel–Kekulé-VBS order is shown to be a nonlinear sigma model augmented by a well-known Wess–Zumino–Witten (WZW) topological term.[41–46] We find that the WZW term leads to a mutual duality for the Néel–Kekulé-VBS transition and that this mutual duality can be realized by a mutual Chern–Simons (CS) theory. We also find that spin–charge separation arises as a consequence of the mutual duality. According to a specific study by Senthil *et al.*[10] and a more general study by Xu,[47] the Néel–Kekulé-VBS transition is associated with an emergent spinon and a gauge field at the critical point, so the transition is indeed a deconfined QCP.

In fact, the treatment of Néel–Kekulé-VBS duality in this paper overlaps partly with some important work by Senthil,[10] Hu,[43] Hosur,[37] and Xu.[47] However, we believe that we offer some new results, especially the origin of the duality in the presence of a mutual CS term and the appearance of dual topological excitations at the boundary between two ordered phases where a QCP may exist. Dual descriptions have also been used in the context of doped Mott insulators for dealing with disordered–ordered phase transitions.[48] A mutual CS term also arises in the theory of spin-$1/2$ quantum magnets[47] and doped antiferromagnets,[49–51] but with the slight difference that the mutual CS theory there originates from the spin and charge sectors, whereas here the mutual CS term requires only the presence of mutual topological excitations. We must point out, however, that we have considered a continuous symmetry in this paper, and whether dual topological excitations exist for discrete symmetries remains an open problem.

The remainder of this paper is organized as follows. In Section 2, we define the general GNY term and solve the uniform critical coupling for possible broken orders. In Section 3, we study quantum criticality in the vicinity of the typical Néel–Kekulé-VBS transition. In this section, we also derive the WZW action for a five-component Néel–Kekulé-VBS order vector and discuss the Néel–Kekulé-VBS mutual duality. In Section 4, we study the derived phenomena at the level of dual topological excitations. Finally, in Section 5, we present a discussion of our results and our conclusions.

2. General Yukawa interactions and mass gap

The graphene semimetal contains two sets of triangular sublattices, denoted by (A,B). Near the two inequivalent Dirac points (K,K') in momentum space, the Hamiltonian for spinless graphene can be written as $H=\sum_k \psi_k^\dagger h(k)\psi_k$, with a single-particle Hamiltonian $h(k)$ of the form (setting the fermion velocity $v_\mathrm{F}=1$ and the reduced Planck constant $\hbar=1$)

$$h(k)=\sum_{i=1,2}\alpha_i k_i,\quad \alpha_1=-\tau_3\otimes\sigma_2,\quad \alpha_2=\tau_3\otimes\sigma_1, \tag{1}$$

where the 2×2 unit matrix τ_0 and the Pauli matrices τ_i $(i=1,2,3)$ act on the valley indices (K,K'), while the 2×2 unit matrix σ_0 and the Pauli matrices σ_i $(i=1,2,3)$ act on the sublattice indices (A,B). In this representation, the four-component spinor ψ_k around the Dirac nodes is given by $\psi_k=(c_{KA},c_{KB},c_{K'B},c_{K'A})^\mathrm{T}$.

Now, let us define the mass matrix in the Hamiltonian. The general two-dimensional Dirac Hamiltonian is

$$H=\alpha_1 k_1+\alpha_2 k_2+\Delta\mathcal{M}, \tag{2}$$

where $\mathcal{M}$ is a matrix satisfying $\mathcal{M}^2=\mathbb{I}$ and the anticommutation relations $[\alpha_{1,2},\mathcal{M}]_+=0$, and Δ is a parameter with a mass scale. These relations lead to a gapped fermionic spectrum of the form $E_k=\pm\sqrt{\boldsymbol{k}^2+\Delta^2}$. Therefore, we say that Δ is the mass gap of the massive Dirac particle, and $\mathcal{M}$ is the mass matrix, which plays the role of a parameter for the insulating phases. For example, $\mathcal{M}=\tau_0\otimes\sigma_3$ is the mass matrix of the integer quantum Hall effect, which can be seen explicitly by writing $\psi_k^\dagger\tau_0\otimes\sigma_3\psi_k$ in the Dirac Hamiltonian. To describe the rich ground states of electrons within the uniform framework of the Dirac equation, we can introduce the unit matrix s_0 and another set of Pauli matrices s_i $(i=1,2,3)$ which act on the spin indices. Taking spin, valley and sublattice degrees of freedom into account, the eight-component spinor is given by $\Psi=(\psi_{k\uparrow},\psi_{k\downarrow})^\mathrm{T}$, where $\psi_{k\uparrow}$ (or $\psi_{k\downarrow}$) is a four-component spinor that acts on the combined space of valley and sublattice degrees of freedom. Then, the eight-dimensional representation of the α_i $(i=1,2)$ matrices can be constructed as $\alpha_1=s_0\otimes(-\tau_3)\otimes\sigma_2$ and $\alpha_2=s_0\otimes\tau_3\otimes\sigma_1$. In the eight-dimensional representation, we define the general mass matrix $\mathcal{M}_{\mu\nu\lambda}=s_\mu\otimes\tau_\nu\otimes\sigma_\lambda$, which must anticommute with α_i $(i=1,2)$.

Having defined the mass matrix, we now turn to the field-theoretical description of mass generation in the semimetal–insulator transition. It is convenient to start with an effective action that includes a general four-fermion interaction and is defined by

$$S(\bar\psi,\psi)=\int \mathrm{d}^3x\left[\bar\psi\gamma^\mu \mathrm{i}\partial_\mu\psi+\frac{g}{2}(\bar\psi\mathcal{M}\psi)^2\right], \tag{3}$$

where g labels the coupling strength for four-fermion interactions. In this action, the four-component spinors $\bar\psi$ and ψ are independent Grassmann variables and depend on the $(2+1)$-dimensional spacetime (t,x,y). We have defined the gamma matrices $\gamma^0=\beta=s_0\otimes\tau_0\otimes\sigma_3$, $\gamma^1=\beta\alpha_1=s_0\otimes\tau_3\otimes(\mathrm{i}\sigma_1)$, $\gamma^2=\beta\alpha_2=s_0\otimes\tau_3\otimes(\mathrm{i}\sigma_2)$, and $\bar\psi\equiv\psi^\dagger\gamma^0$. To define the

projection operator $P=(1\pm\gamma^5)/2$, we need another gamma matrix $\gamma^3=\beta\alpha_3=s_0\otimes\tau_3\otimes\sigma_0$ such that $\gamma^5=-\mathrm{i}\gamma^0\gamma^1\gamma^2\gamma^3=s_0\otimes\tau_3\otimes\sigma_0$ is diagonal. We have also defined the fermion bilinear in terms of the general mass matrix in the Lagrangian. This model is similar to the Gross–Neveu model with discrete chiral symmetry that is used to discuss the dynamical mass of gauged vector mesons in particle physics. Mass generation can be studied by rewriting the functional integral as

$$Z=\int\mathcal{D}[\bar\psi,\psi,\phi]\,\mathrm{e}^{\mathrm{i}S(\bar\psi,\psi,\phi)},$$
$$S(\bar\psi,\psi,\phi)=\int\mathrm{d}^3x\left[\bar\psi(\gamma^\mu\mathrm{i}\partial_\mu-\phi\mathcal{M})\psi-\frac{\phi^2}{2g}\right]. \quad (4)$$

The decoupling of the four-fermion interaction by the introduction of an auxiliary boson field in the functional integral is known as the Hubbard–Stratonovich transformation, and this leads to the general GNY interactions. Equation (4) shows that $\mathcal{M}$ plays the role of a mass matrix and thus corresponds to an order pattern. To study the ground-state behavior, we consider the static boson field. Integrating over the fermion fields, we obtain the effective potential for the boson field

$$V_{\mathrm{eff}}(\phi)=\frac{\phi^2}{2g}+\frac{\mathrm{i}}{(2\pi)^3}\ln\left[\det(\gamma^\mu\mathrm{i}\partial_\mu-\phi\mathcal{M})\right]. \quad (5)$$

We have found that the determinant $\det(\gamma^\mu\mathrm{i}\partial_\mu-\phi\mathcal{M})$ depends only on the dimension of the mass matrix and is independent of its particular form, $\det(\gamma^\mu\mathrm{i}\partial_\mu-\phi\mathcal{M})=(k^2-\phi^2)^{D/2}$. Then, the effective potential is given by

$$\begin{aligned}V_{\mathrm{eff}}(\phi)&=\frac{\phi^2}{2g}+\frac{\mathrm{i}}{(2\pi)^3}\int\mathrm{d}^3k\ln(k^2-\phi^2)^{D/2}\\&=\frac{\phi^2}{2g}-\frac{D}{4\pi^2}\int_c^\phi\mathrm{d}\phi^2\left(\Lambda-\frac{\phi^2}{2}\ln\frac{\Lambda^2+\phi^2}{\phi^2}\right), \quad (6)\end{aligned}$$

where Λ is the ultraviolet cutoff in the regularization, D is the dimension of the mass matrix, and we have introduced an arbitrary constant c in the integral. We would like to find the nonzero expectation value of the boson field due to spontaneous symmetry breaking. For our purposes, it is convenient to derive the gap equation by minimizing the potential (i.e., putting $\partial V_{\mathrm{eff}}/\partial\phi=0$)

$$\frac{1}{g(\Lambda)}=\frac{4}{\pi^2}\int_0^\Lambda\frac{k_{\mathrm{E}}^2\,\mathrm{d}k_{\mathrm{E}}}{k_{\mathrm{E}}^2+\phi^2}, \quad (7)$$

where we have used the Euclidean variable k_{E}. This equation yields the critical coupling strength $g_{\mathrm{c}}=\pi^2/4\Lambda$ for the general GNY interactions; this is one of the main results of this paper. It is worth noting that Sato *et al.*[29] have numerically shown the existence of a tricritical point for Néel–Kekulé-VBS, and semimetallic phases in a honeycomb lattice with some emergent symmetries. When $g(\Lambda)>g_{\mathrm{c}}$, the symmetry breaking leads to an insulating phase, and the nonzero ϕ is the mass gap. To confirm the fermion mass gap, setting $\phi=\phi(\Lambda,g)$, we find the flow equation

$$\frac{\partial g(\Lambda)}{\partial\Lambda}=-\frac{4g^2(\Lambda)}{\pi^2}\left(1-\frac{\Lambda\phi^2}{\Lambda^2+\phi^2}\right). \quad (8)$$

Moreover, the mass gap satisfies

$$\left(\Lambda\frac{\partial}{\partial\Lambda}+\beta(g)\frac{\partial}{\partial g}\right)\phi=0,\quad \beta(g)=\Lambda\frac{\partial g}{\partial\Lambda}. \quad (9)$$

This means that the mass gap is irrelevant to the cutoff Λ and the running coupling g, and thus the fermion mass term is a renormalization-group invariant.

Finally, we point out that the general fermion bilinear can be represented as $\psi^\dagger\mathcal{M}\psi$, modulation of which will lead to an insulating phase. For example, Kekulé distortion and Kekulé-VBS are modulations of nearest-neighbor hopping bonds with different sublattices and Dirac nodes,

$$c_{kA}^\dagger c_{k'B}+c_{kB}^\dagger c_{k'A}+c_{k'B}^\dagger c_{kA}+c_{k'A}^\dagger c_{kB}, \quad (10)$$
$$-\mathrm{i}c_{kA}^\dagger c_{k'B}-\mathrm{i}c_{kB}^\dagger c_{k'A}+\mathrm{i}c_{k'B}^\dagger c_{kA}+\mathrm{i}c_{k'A}^\dagger c_{kB}. \quad (11)$$

The mass matrices corresponding to these modulations are $\mathcal{M}_{010}$ and $\mathcal{M}_{020}$, which serve as the order parameters of real VBS ($\Re$VBS) and imaginary VBS ($\Im$VBS), respectively. The Néel orders (N_x,N_y,N_z) correspond to the modulation of the fermion bilinear with staggered magnetization, and the mass matrix can be represented as $\mathcal{M}_{133}$, $\mathcal{M}_{233}$, $\mathcal{M}_{333}$. Besides, the microscopic orders for the fermion bilinear with two lattice fermions sitting on the same sublattice include charge density waves (CDWs), the quantum Hall effect (QHE) and the spin–orbit coupling-driven quantum spin Hall effect (QSHE). We enumerate these common fermion bilinears in Table 1.

Table 1. Common mass matrices $\mathcal{M}$ and corresponding order parameters $\mathcal{O}$. Here we list the typical Kekulé-VBS phase, Néel phase, quantum Hall effect phase, quantum spin Hall effect phase and charge density wave phase. The subscript $i=x,y,z$ denotes the spin-s_i projected order parameter, and $\Re\mathcal{O}$ and $\Im\mathcal{O}$ are the real and imaginary order parameters, respectively.

$\mathcal{O}$	$\mathcal{M}$	$\mathcal{O}$	$\mathcal{M}$
$\Re$VBS	$s_0\otimes\tau_1\otimes\sigma_0$	QHE	$s_0\otimes\tau_0\otimes\sigma_3$
$\Re\mathrm{VBS}_x$	$s_1\otimes\tau_1\otimes\sigma_0$	QSHE_x	$s_1\otimes\tau_0\otimes\sigma_3$
$\Re\mathrm{VBS}_y$	$s_2\otimes\tau_1\otimes\sigma_0$	QSHE_y	$s_2\otimes\tau_0\otimes\sigma_3$
$\Re\mathrm{VBS}_z$	$s_3\otimes\tau_1\otimes\sigma_0$	QSHE_z	$s_3\otimes\tau_0\otimes\sigma_3$
$\Im$VBS	$s_0\otimes\tau_2\otimes\sigma_0$	CDW	$s_0\otimes\tau_3\otimes\sigma_3$
$\Im\mathrm{VBS}_x$	$s_1\otimes\tau_2\otimes\sigma_0$	$\mathrm{Néel}_x$	$s_1\otimes\tau_3\otimes\sigma_3$
$\Im\mathrm{VBS}_y$	$s_2\otimes\tau_2\otimes\sigma_0$	$\mathrm{Néel}_y$	$s_2\otimes\tau_3\otimes\sigma_3$
$\Im\mathrm{VBS}_z$	$s_3\otimes\tau_2\otimes\sigma_0$	$\mathrm{Néel}_z$	$s_3\otimes\tau_3\otimes\sigma_3$

3. Néel–Kekulé-VBS duality

We have seen in Section 2 that there exists a multicritical point that separates the semimetallic phase and the insulating phases. Among these insulating phases, the mass matrices that anticommute pairwise are not competing, while the mass matrices that commute pairwise are competing.[36] If there are

two phases that do not compete with each other, it is possible to adiabatically change one phase into another without closing the fermion gap. For example, the mass matrices for the Néel and Kekulé-VBS phases are not competing, so the phase transitions between them may be continuous.

In the vicinity of the Néel–Kekulé-VBS crossing line, the two ordered phases break different symmetries. Suppressing one phase will automatically lead to the emergence of the other phase. As shown in Ref. [47], the concept of defect condensation is appropriate when discussing such phase transitions. It is well known that the $SO(5)$ superspin nonlinear sigma model (NLSM) with the extra topological WZW term of a quantum spin-$1/2$ magnet precisely reproduces the same power law and long-distance correlations for both the Néel and VBS order parameters.[43,46] The WZW term represents the mutual property of the superspin (Néel-VBS) order parameters with its hidden symmetry. The Néel and Kekulé-VBS mass matrices anticommute with each other and so form a five-tuplet of compatible mass matrices.[36] In Ref. [37], it was shown that a topological "hedgehog" configuration (a point topological defect) carries a single zero mode at its core, and in the background of the Néel–Kekulé-VBS five-tuplet, a defect-driven continuous phase transition becomes possible.

In what follows, we derive the WZW term[41–46] for the Néel–Kekulé-VBS order parameters. To our knowledge, although a similar WZW term has been derived in a Fermi system,[37] no study of the Néel–Kekulé-VBS transition in Dirac semimetals within the WZW formalism has previously been published. We will see that the WZW term yields a mutual duality between two ordered phases, which may play an important role in continuous quantum criticality. The Néel–Kekulé-VBS five-tuplet is composed of the three-component Néel vector and the doublet (real and imaginary) of VBS order parameters

$$\vec{\phi} \equiv (\vec{N}, \Re\mathrm{VBS}, \Im\mathrm{VBS}). \tag{12}$$

This five-tuplet supports a quasiparticle excitation with $SU(2)$ (spin rotation) and $U(1)$ (rotation between real and imaginary Kekulé-VBS order parameters) symmetry. In $(2+1)$-dimensional spacetime, the $SU(2)\times U(1)$ vector (defined on the surface S^4) has no topologically nontrivial configurations, since $\pi_3(S^4)=0$; that is, there are no topological excitations. However, it does support topological excitations perturbatively, owing to the nontrivial homotopy group $\pi_4(S^4)=\mathbb{Z}$, which yields the WZW term. We now consider the action

$$S[\psi,\bar{\psi},\vec{n}] = \int \mathrm{d}^3x\, \bar{\psi}(\mathrm{i}\gamma^\mu\partial_\mu - \Delta\Upsilon^l n_l)\psi, \tag{13}$$

where $\vec{n}=\vec{\phi}/|\vec{\phi}|$, $\vec{N}^2=n_1^2+n_2^2+n_3^2$, $\Delta_{\mathrm{VBS}}^2=n_4^2+n_5^2$, $\Upsilon^l=\gamma_0\mathcal{M}_l$, and $\mathcal{M}_l$ is the Néel–Kekulé-VBS mass matrix. It is obvious that this action reproduces the general Dirac Hamiltonian (2). The WZW terms can be restored perturbatively by integrating over the Dirac fermions in the background of the slowly varying Néel–Kekulé-VBS five-tuplet. Following the spirit of Abanov and Wiegmann,[45] the effective action for the Néel–Kekulé-VBS five-tuplet can be obtained as

$$\begin{aligned} \mathrm{e}^{\mathrm{i}S(\vec{n})} &= \int \mathcal{D}[\psi,\bar{\psi}]\,\mathrm{e}^{-S(\bar{\psi},\psi,\vec{n})}, \\ S(\vec{n}) &= -\mathrm{i}\,\mathrm{Tr}\ln(\mathrm{i}\gamma^\mu\partial_\mu - \Delta\Upsilon^l n_l). \end{aligned} \tag{14}$$

The perturbative expansion gives the leading action (see Ref. [37] or Appendix A) $S(\vec{n})=S_0(n_l)+S^{\mathrm{E}}_{\mathrm{WZW}}(\vec{n})$, with

$$S_0(n_l) = \frac{1}{g}\int \mathrm{d}^3x(\partial_\alpha n_l)^2, \quad \frac{1}{g}\sim\Delta, \tag{15}$$

$$\begin{aligned} S^{\mathrm{E}}_{\mathrm{WZW}}(\vec{n}) = {} & \frac{4\pi\mathrm{i}}{4!\,\mathrm{Area}(S^4)}\epsilon^{\alpha\beta\tau\rho}\epsilon^{abcde}\int \mathrm{d}^2x\,\mathrm{d}\tau\int_0^1 \mathrm{d}\rho \\ & \times(\partial_\alpha n_a)(\partial_\beta n_b)(\partial_\tau n_c)(\partial_\rho n_d)n_{\mathrm{e}}. \end{aligned} \tag{16}$$

The appearance of the WZW term $S^{\mathrm{E}}_{\mathrm{WZW}}(\vec{n})$ gives rise to the Néel–Kekulé-VBS duality, which implies that the topological objects of one phase carry the quantum number of the other phase (see below for details).

The Néel order breaks $SU(2)$ spin rotation symmetry to a $U(1)$ symmetry, and the $O(3)$ vector $\vec{n}=(n_1,n_2,n_3)$ for the Néel order should then be defined on a sphere. The Kekulé-VBS breaks C_6 lattice rotation or lattice translational symmetry, and if we consider the complex Kekulé-VBS order parameter, then the discrete symmetry can be enlarged to an enhanced $U(1)$ symmetry. As discussed in the context of the superfluid phase transition or the XY model, for a symmetry-unrelated phase transition, each ordered phase can be driven by condensation of the topological defects of the ordered phase.[47] We adopt the $\mathbb{C}P^1$ parametrization $n_a=z^\dagger\sigma_a z$, where $z=(z_1,z_2)^{\mathrm{T}}$ is a complex two-component spinor with the constraint $|z_1|^2+|z_2|^2=1$, and $z_{1,2}$ are fractionalized "spinon" fields. We observe the skyrmion charge in the Néel order as a total gauge flux quantum

$$q_{\mathrm{s}} = \frac{1}{4\pi}\epsilon^{ij}\vec{n}\cdot(\partial_i\vec{n}\times\partial_i\vec{n}) = \frac{1}{2\pi}\int \mathrm{d}^2x\,\epsilon^{ij}\partial_i a_j, \tag{17}$$

where $a_i=-\frac{1}{2}\mathrm{i}(z^\dagger\partial_i z-\partial_i z^\dagger z)$. The skyrmion is mapped exactly to a "magnetic" flux quantum. The internal gauged $U(1)$ symmetry appears as $a_j\to a_j+\partial_j f$, so the skyrmion number is conserved. Since the Kekulé-VBS order parameter preserves $U(1)$ symmetry, it supports a topological defect in the form of a vortex. In the dual description of vortex defects in the Kekulé-VBS order, the vorticity plays the role of an"electric" charge

$$q_{\mathrm{v}} = \int_c \mathrm{d}l\,\partial_i e_i = \int_c \mathrm{d}l\,\epsilon^{ij}\partial_i\partial_j a_0. \tag{18}$$

In this case, the scalar field a_0 is the phase field, and therefore the Néel and Kekulé-VBS orders are dual to each other owing to electromagnetic duality.

Because the Néel order preserves a $U(1)$ gauge degree of freedom after $SU(2)$ is broken, the spinon field z_α will be coupled to the dynamical $U(1)$ gauge field a_μ, and we obtain the $\mathbb{C}P^1$ model $S_z = \int \mathrm{d}^2x\mathrm{d}\tau L_z$, which describes the deconfined QCP between the Néel and Kekulé-VBS orders[10]

$$L_z = |(\partial_\mu - \mathrm{i}a_\mu)z_\alpha|^2 + s_z|z_\alpha|^2 + r_z|z_\alpha|^4 + \kappa(\epsilon^{\mu\nu\lambda}\partial_\nu a_\lambda)^2, \quad (19)$$

where s_z and r_z are parameters similar to those in ϕ^4 theory, and κ is a constant. The study of the critical point can be aided by introducing a matter field and a gauge field b_μ for the vortex defect in the Kekulé-VBS order. Once the matter fields have condensed, the gauge field acquires a mass term b_μ^2 via the Higgs mechanism. We can then derive (after integrating over b_μ) the Maxwell term in L_z by incorporating the mutual CS term[49]

$$L_{\mathrm{mcs}} = \mathrm{i}\sqrt{2\kappa}\,\epsilon^{\mu\nu\lambda}b_\mu\partial_\nu a_\lambda. \quad (20)$$

The mutual CS term is the concentrated reflection of the mutual duality between the Néel and Kekulé-VBS orders. Under the gauge transformation $b_\mu \to b_\mu + \partial_\mu f^b$, the current is given by $j_\mu^a = \mathrm{i}\sqrt{2\kappa}\,\epsilon^{\mu\nu\lambda}\partial_\nu\partial_\lambda f^b$, and the time component represents the Kekulé-VBS vortex when f^a sweeps across the singularity of the vortex in the Kekulé-VBS order. Thus, the charge–vortex duality is captured by the mutual CS term or the WZW term in terms of the Néel–Kekulé-VBS order vector.

We should stress that a mutual CS term has also been derived for a $\mathbb{Z}_2$ spin liquid and a doped Mott insulator via a decomposition of the electron charge and spin degrees of freedom, as for a high-T_c superconductor.[40,49] In the present paper, however, the presence of the mutual CS term depends on the existence of dual topological excitations at the two sides of a critical boundary. The skyrmion and vortex configurations relate to a continuous symmetry, and extension to topological configurations with a discrete symmetry remains an interesting topic for future study.

Let us turn to describing the phase transition. As shown in Eq. (17), the skyrmion is conserved, and it corresponds to the configuration of a_μ that creates a 2π flux. Once the quantum flux has condensed, the extra term induced by the mutual CS term is nonvanishing; i.e., $\int \mathrm{d}^2x\mathrm{d}\tau\,\epsilon^{\mu\nu\lambda}\partial_\mu f^b\langle\partial_\nu a_\lambda\rangle \neq 0$. The flux condensation destroys the skyrmion number; meanwhile, it spontaneously breaks the $U(1)_b$ symmetry and leads to the Kekulé-VBS order. Condensation of the vortex in the Kekulé-VBS order gives $\langle b_\mu\rangle \neq 0$, but this condensation has no effect on the gauge condition $\int \mathrm{d}^2x\mathrm{d}\tau\,\epsilon^{\mu\nu\lambda}\partial_\nu\partial_\lambda f^a\langle b_\mu\rangle = 0$, and it does not destroy the conservation law

$$\partial_\mu j_a^\mu = 0. \quad (21)$$

The spinon fields z_α preserve the $U(1)_a$ symmetry, and their condensation is defined on the surface of a two-dimensional sphere, which is equivalent to the Néel order.[47] The spinons emerge at the critical point, so the Néel–Kekulé-VBS transition is a deconfined QCP. Such QCPs may be generalized to other multiple-component order vectors.

From the above discussion, it can be seen that the compatible mass matrices generate a continuous quantum criticality between the Néel and Kekulé-VBS transitions. It was shown in Refs. [36] and [37] that as a result of quantum fluctuations of the massless Dirac fermions, the semimetal–insulator transition with emergent symmetries (e.g., $\mathbb{Z}_3$ and $\mathbb{Z}_2$) is continuous. We can therefore conclude that the semimetal–insulator transition with some emergent symmetries may be continuous, and may thus exhibit a new class of critical point. It is worth noting that Jian and Yao[52] have studied the Gross–Neveu criticality between a Dirac semimetal and a gapped insulator which breaks $\mathbb{Z}_2$ symmetry.

4. Dual topological excitations

In this section, we study the mutual duality at the level of static topological excitations. We will see that the phenomenon of spin–charge separation results from the Néel–Kekulé-VBS mutual duality. In addition, we obtain a formula for the index theorem in terms of the mutual duality.

The WZW term exhibits the mutual duality between Néel and Kekulé-VBS orders, and we now turn our attention to the connections between duality and emergent phenomena, such as fractionalized quasiparticles and spin–charge separation. The Kekulé-VBS order pattern corresponds to modulation of the fermion bilinear operator with different sublattices and Dirac points, and thus preserves chiral symmetry. When the fermion spinor ψ occurs in the Kekulé-VBS mass matrix, the mass matrix $V_{ab} = \psi^\dagger\mathcal{M}_{ab}\psi$ acquires a nonzero value (without spin degrees of freedom being taken into account); for instance,

$$\langle V_{10}\rangle = \Delta\left\langle\psi^{\mathrm{T}}\tau_1\otimes\sigma_0\psi\right\rangle \neq 0, \quad (22)$$

and such condensates gap-out the nodal quasiparticles. It is known that a static background can support zero-mode quasiparticles. To demonstrate the connection between the twisted Kekulé-VBS order and mid-gap zero energy states at the level of the fermionic spectrum, it is convenient to assume that the order pattern is slowly varying on the scale of the lattice spacing and that the nontrivial background topology will be realized by a complex-valued mass matrix field. In the continuum limit, we write the complex Kekulé-VBS mass matrix as $V = \Re V + \mathrm{i}\Im V$, with $\Re V = \Delta\left\langle\psi^{\mathrm{T}}\tau_1\otimes\sigma_0\psi\right\rangle$ and $\Im V = -\mathrm{i}\Delta\left\langle\psi^{\mathrm{T}}\tau_2\otimes\sigma_0\psi\right\rangle$. In polar coordinates, the Lagrangian of the fermion interacting with the twisted Kekulé-VBS order parameter reads

$$L_{\mathrm{VBS}} = \bar\psi\gamma^\mu(\mathrm{i}\partial_\mu + \gamma_5 a_{5\mu})\psi - \bar\psi\Delta\beta V\psi, \quad (23)$$

$$V = \beta_1\cos\theta + \beta_2\sin\theta, \quad (24)$$

where $\beta=\tau_0\otimes\sigma_3$, $\beta_1=\tau_1\otimes\sigma_0$, and $\beta_2=\tau_2\otimes\sigma_0$ are the real and imaginary Kekulé-VBS mass matrices, respectively. We have also performed a polar decomposition of the mass matrix in Eq. (24). There is a local gauge symmetry

$$\psi'=\mathrm{e}^{\mathrm{i}\omega\gamma_5}\psi,\quad a'_{5\mu}=a_{5\mu}+\partial_\mu\omega,\quad \Delta'=\Delta\mathrm{e}^{\mathrm{i}\omega\gamma_5}, \tag{25}$$

where ω is a real number and $\mu=t,x,y$, and we have also chosen a gauge potential with vanishing temporal component. The phase twist in the Kekulé-VBS mass matrix leads to a domain wall or vortex in two spatial dimensions; indeed, the background topology for the Lagrangian is equivalent to that of the Jackiw–Rossi model that describes a charged fermion interacting with the scalar fields of the two-dimensional Abelian Higgs model.

There have been many studies of single-valued and normalizable wavefunctions for zero-energy solutions in the presence of nontrivial twist fields. For an n-twisted order parameter, there are n independent normalizable zero-energy states, and the properties and the specific forms of each zero-energy solution may differ. The Hamiltonian subject to the Kekulé-VBS order pattern is given by

$$H=\alpha_i(-\mathrm{i}\partial_i-\gamma_5 a_{5i})+\Delta(r)(\beta_1\cos\theta+\beta_2\sin\theta), \tag{26}$$

and the normalizable zero-energy solutions can be found in Appendix B. When the degree of twisting of the Kekulé-VBS order is equal to $2k$ ($k\in N$), there are $2k$ normalizable zero modes, and each zero-energy mode is characterized by two phases, $\psi_{ka}=f\mathrm{e}^{\mathrm{i}l_1\theta}+g\mathrm{e}^{\mathrm{i}l_2\theta}$ ($l_1\neq l_2$, $l_1,l_2\in N$); when the degree of twisting is equal to $2k+1$, there are $2k+1$ zero modes, among which only one is single-phase dependent ($l_1=l_2$), while the others are two-phase dependent. In polar coordinates, the normalizable single-phase dependent wavefunction for zero modes on sublattice A can easily be obtained as

$$\begin{aligned}\psi_{kA}&=\mathcal{N}_A\exp\left\{-\int_0^r\left[\Delta(r)+\frac{2na_5(r)-(n-1)}{2r}\right]\mathrm{d}r\right\}\\&\quad\times\exp\left\{\mathrm{i}\left[\frac{(n-1)\theta}{2}-\frac{\pi}{4}\right]\right\},\\\psi_{k'A}&=\mathrm{i}\bar{\psi}_{kA},\end{aligned} \tag{27}$$

where $\mathcal{N}_A$ is a normalization coefficient. Since $\Delta(r)$ and $a_5(r)$ vanish at small r, for the wavefunction to be normalizable, it is necessary that $n\leq-1$. Similarly, the normalizable single-phase dependent zero mode on sublattice B is

$$\begin{aligned}\psi_{kB}&=\mathcal{N}_B\exp\left\{-\int_0^r\left[\Delta(r)+\frac{(n+1)-2na_5(r)}{2r}\right]\mathrm{d}r\right\}\\&\quad\times\exp\left\{\mathrm{i}\left[\frac{(n+1)\theta}{2}+\frac{\pi}{4}\right]\right\},\\\psi_{k'B}&=-\mathrm{i}\bar{\psi}_{kB},\end{aligned} \tag{28}$$

where $\mathcal{N}_B$ is a normalization coefficient. For the wavefunction at small r to be normalizable, it is necessary that $n\geq1$; the normalizability condition can also be found in Ref. [53]. Owing to the sublattice symmetry (or the chiral symmetry), the zero-mode wavefunction on sublattice A also holds on sublattice B, with the substitutions $\psi_{ka}\to\psi_{kb}$ and $n\to-n$. The sublattice symmetry ensures that the energy eigenstates $\pm E$ come in pairs, and thus the zero modes bound to the VBS vortex are classified by $\mathbb{Z}_2$. Only for odd twisting is there at least one topologically protected fermion zero mode. In Ref. [37], it was shown that there exist zero-energy modes in the core of the Néel "hedgehog" and that the five-component vector of Néel–Kekulé-VBS order parameters forms a five-tuplet, and so dual topological excitations can exist at the boundary of two symmetry-unrelated phases.

As shown above, the Kekulé-VBS order exhibits spectral reflection symmetry, and the vortex defect hosts a single fermionic mid-gap zero-energy mode in the core. To make the Néel–Kekulé-VBS duality explicit, follow the same approach as in Ref. [37], and use the five-component Néel–Kekulé-VBS order parameter ansatz

$$\vec{n}=\left[\sqrt{1-\phi^2(r)}\vec{s}(\tau,\rho),\phi(r)\vec{v}\right], \tag{29}$$

where $\phi(0)=0$ and $\phi(\infty)=1$, and $\vec{v}$ encodes the defect core. Integrating over space leads to the effective action in the vicinity of the core of the vortex defect

$$S^{\mathrm{v}}=\frac{\mathrm{i}}{4}\int\mathrm{d}\tau\mathrm{d}\rho\,\epsilon^{\alpha\beta}\epsilon^{abc}s_a(\partial_\alpha s_b)(\partial_\beta s_c), \tag{30}$$

which is precisely the WZW term for a spin $1/2$ in $(0+1)$ dimension, i.e., a $1/2$-spinon. Therefore, the vortex defect carries the $1/2$-spinon quantum number. Kramers conjugation ensures that there are two zero-energy levels for time-reversal-symmetric systems, each carrying an up $1/2$-spinon quantum number and a down $1/2$-spinon quantum number, respectively. The occupation pattern of these zero modes yields two charged states and two spinon states: $(\Delta Q=1,S_z=0)$, $(\Delta Q=-1,S_z=0)$, $(\Delta Q=0,S_z=1/2)$, $(\Delta Q=0,S_z=-1/2)$, where ΔQ is the total charge and S_z is the total spin. These states are precisely the spin–charge separation holon, the chargeon, and the two spinon states studied in the QSHE.[54,55] Therefore, we see spin–charge separation as consequences of duality. Moreover, the condensation of these bosons and spinons may be helpful for understanding the rich variety of phase transitions such as the spin-liquid–magnetic and superconductor–magnetic transitions.

The index theorem establishes a link between topological stability and the number of zero modes from Eq. (26), by relating the analytical index of a Dirac operator to the winding number of the Kekulé-VBS background scalar field in two spatial dimensions.[56,57] In addition to any symmetries, we now show that the Néel–Kekulé-VBS duality provides an alternative way to derive the topological index. We consider a model

with fermions interacting with the complex Kekulé-VBS order. The dual target space can be obtained by considering the extended Kekulé-VBS order parameter $\phi = (\Re\Delta, \Im\Delta, h)$, according to the Lagrangian density

$$L = \bar{\psi}\mathrm{i}\gamma^{\mu}(\partial_{\mu} - \mathrm{i}\gamma_5 a_{5\mu})\psi - \bar{\psi}\left(\sum_{k=1}^{3}\Gamma_k\phi_k\right)\psi, \tag{31}$$

where $\Gamma_k = \beta(\beta_1, \beta_2, \mathbb{I})$ and we have introduced an auxiliary parameter $-\infty < h < \infty$. The extended order parameter defines a topological current (see Appendix C)

$$J^{\mu} = -\frac{1}{8\pi\phi^3}\epsilon^{\mu\nu\lambda}\epsilon^{abc}\phi_a\partial_{\nu}\phi_b\partial_{\lambda}\phi_c, \tag{32}$$

and the index for the vortex can be derived by regularizing $h = 0$. We assume that the Kekulé-VBS vortex $(\Re\Delta, \Im\Delta)$ lies on the plane $h = 0$. The half-degree can be separated into two parts

$$\Omega/2 = \int \mathrm{d}^2x\,[J^0(a=3) + J^0(a\neq 3)]. \tag{33}$$

It can easily be shown that the second term vanishes when h is regularized to zero. The half-degree of the mapping then becomes

$$\Omega/2 = -\int \mathrm{d}^2x\,\epsilon^{ij}\epsilon^{ab}h\partial_i\phi_a\partial_j\phi_b/8\pi\phi^3. \tag{34}$$

In polar coordinates, $\phi = \Delta(r)\hat{\phi}(\theta)$, where $\hat{\phi} = \phi_i/|\phi|$ $(i = 1,2,3)$, and the half-degree of the mapping is given by

$$\begin{aligned}\Omega/2 &= -\frac{1}{4\pi}\int_0^{\infty}\frac{h\,\mathrm{d}(\Delta^2)}{(\Delta^2+h^2)^{3/2}}\int \mathrm{d}\theta\,\epsilon^{ab}\hat{\phi}_a\partial_{\theta}\hat{\phi}_b \\ &= \frac{1}{4\pi}\int \mathrm{d}\theta\,\epsilon^{ab}\hat{\phi}_a\partial_{\theta}\hat{\phi}_b.\end{aligned} \tag{35}$$

We thus obtain the well-known result

$$\Omega = \frac{1}{2\pi}\int \mathrm{d}\theta\,\epsilon^{ab}\hat{\phi}_a\partial_{\theta}\hat{\phi}_b. \tag{36}$$

Without the need for any symmetry considerations, this result has been deduced from the Néel–Kekulé-VBS duality. We know that this number also gives the difference between the number of zero modes with opposite chirality. Thus, the duality in the vicinity of the critical point implies an associated mapping between the target spaces of the topological excitations. Taking this into account, the Néel–Kekulé-VBS duality implies that there exists an invariant related to the theories represented by the following two Lagrangians:

$$L_1 = \bar{\psi}\mathrm{i}\gamma\cdot(\partial - \mathrm{i}\gamma_5 a)\psi + m(r)\mathrm{e}^{\mathrm{i}\gamma_5\theta}\bar{\psi}\psi + \cdots, \tag{37}$$

$$L_2 = \bar{\psi}\mathrm{i}\gamma\cdot(\partial - \mathrm{i}b)\psi + \bar{\psi}\vec{n}\cdot\vec{\sigma}\psi + \cdots. \tag{38}$$

5. Conclusion and discussions

In summary, we have found that a moderate four-fermion interaction leads to a multicritical point for various insulating phases in Dirac semimetals and that this represents a non-Landau transition. We have also studied the typical Néel–Kekulé-VBS quantum criticality, for which the compatible Néel–Kekulé-VBS five-tuplet leads to a WZW term, and this in turn yields a mutual duality between Néel and Kekulé-VBS orders near the non-Landau critical point. From a static point of view, there is a mutual duality in the sense that a topological defect in either phase carries the quantum number of the other phase, a result that is already well understood.[47] Dynamically, the mutual duality is accompanied by two fluctuating gauged fields, as encoded in the mutual CS term. In this paper, the presence of a mutual CS term is dependent on the existence of dual topological excitations at the boundary of two phases, whereas in the case of a doped Mott insulator, topological excitations in the spin and charge sectors are required for the duality. The compatible mass matrices generate a continuous quantum criticality in the Néel–Kekulé-VBS transition, and the quantum fluctuations render the semimetal–insulator transition with emergent symmetries continuous. Thus, the general semimetal–insulator transition with emergent symmetries may exhibit a new class of critical point. Furthermore, from the perspective of dual topological excitations, spin–charge separation arises as a consequence of mutual duality.

It is worth pointing out that in this paper, Néel–Kekulé-VBS duality refers to self-duality near the critical point, rather than duality between two seemingly different theories. Various recent studies have concentrated on the duality between field theories in high-energy physics and quantum criticality in condensed matter physics, which is a duality in the sense that both theories are described by the same low-energy effective field theory and are characterized by the same critical behavior at criticality. Examples include the duality between noncompact quantum electrodynamics with two flavors ($N_{\mathrm{f}} = 2$) in $2+1$ dimensions (QED_3) and the easy-plane $U(1)$ noncompact $\mathbb{C}P^1$ model[58,59] (describing the Néel–VBS transition in magnets with XY spin symmetry), and the duality between the QED_3–Gross–Neveu model and the $SU(2)$ noncompact $\mathbb{C}P^1$ model.[60]

Generally, we can conclude that there is a hidden duality connecting interacting driven topological quantum phase transitions with quantum criticality, which will contribute to our understanding of fundamental physics.

Appendix A: the nonlinear sigma model with WZW term

The WZW action (16) is the main reason for the existence of the Néel–Kekulé-VBS quantum criticality duality. The effective action can be obtained using a gradient expansion. In

this appendix, we derive the effective theory for the Néel–Kekulé-VBS $SO(5)$ order parameters; a similar derivation can be found in Ref. [37]. In the presence of a slowly varying background, we start from the action

$$S[\psi,\bar{\psi},\vec{n}]=\int \mathrm{d}^3x\,\bar{\psi}(\mathrm{i}\gamma^\mu\partial_\mu-\Delta\Upsilon^l n_l)\psi, \tag{A1}$$

where $\vec{n}=\vec{\phi}/|\vec{\phi}|$, $\Upsilon^l=\gamma_0\mathcal{M}_l$, and $\mathcal{M}_l$ is the Néel–Kekulé-VBS five-component mass matrix. $\Upsilon^1=s_1\otimes\tau_3\otimes\mathbb{I}$, $\Upsilon^2=s_2\otimes\tau_3\otimes\mathbb{I}$, $\Upsilon^3=s_3\otimes\tau_3\otimes\mathbb{I}$, $\Upsilon^4=\mathbb{I}\otimes\tau_1\otimes\sigma_3$, $\Upsilon^5=\mathbb{I}\otimes\tau_2\otimes\sigma_3$, and $\mathbb{I}$ denotes the 2×2 identity matrix. Following the spirit of Abanov and Wiegmann,[45] the effective action for the Néel–Kekulé-VBS order parameter is obtained by integrating over the gapped fermions

$$\begin{aligned}&\mathrm{e}^{\mathrm{i}S_\mathrm{e}[\vec{n}]}=\int\mathcal{D}[\psi,\bar{\psi}]\,\mathrm{e}^{-S[\bar{\psi},\psi,\vec{n}]},\\&S_\mathrm{e}[\vec{n}]=-\mathrm{i}\,\mathrm{Tr}\ln(\mathrm{i}\gamma^\mu\partial_\mu-\Delta\Upsilon^l n_l),\end{aligned} \tag{A2}$$

where Tr here represents the trace over matrix and spatial coordinates. The variation $\delta S_\mathrm{e}[\vec{n}]$ with respect to n_l yields

$$\begin{aligned}\delta S_\mathrm{e}^{(n)}[\vec{n}]&=-\mathrm{i}\,\mathrm{tr}(\mathrm{i}\gamma^\alpha\partial_\alpha-\Delta\Upsilon^a n_a)^{-1}(-\Delta\Upsilon^l\delta n_l)\\&=-\mathrm{i}\sum_n(-1)^n\,\mathrm{tr}\{[(\partial^2+\Delta^2)^{-1}(-\mathrm{i}\Delta\Upsilon^c\gamma^\alpha\partial_\alpha n_c)]^n\\&\quad\times(\partial^2+\Delta^2)^{-1}(-\mathrm{i}\gamma^\beta\partial_\beta-\Delta\Upsilon^s n_s)(-\Delta\Upsilon^l\delta n_l)\},\end{aligned} \tag{A3}$$

where tr here represents the trace over matrix and both spatial and momentum coordinates. It is easily seen that $\delta S_\mathrm{e}^{(1)}[\vec{n}]$ is nonvanishing:

$$\begin{aligned}\delta S_\mathrm{e}^{(1)}[\vec{n}]&=\mathrm{i}\Delta^2\mathrm{tr}[\mathbb{I}_8]\mathrm{tr}_k[(\Delta^2-k^2)^{-2}\partial_\alpha n_l\partial_\alpha\delta n_l]\\&=\frac{\Delta}{2\pi}\int\mathrm{d}^3x\,\partial_\alpha n_l\delta(\partial_\alpha n_l),\end{aligned} \tag{A4}$$

where $k^2=k_0^2-\boldsymbol{k}^2$. $\delta S_\mathrm{e}^{(1)}[\vec{n}]$ yields the $SO(5)$ nonlinear sigma model for the vector $\hat{n}$, which combines the Néel–Kekulé-VBS order parameters

$$S_\mathrm{e}^{(1)}[\vec{n}]=\frac{1}{g}\int\mathrm{d}^3x(\partial_\alpha n_l)^2,\quad\frac{1}{g}\sim\Delta. \tag{A5}$$

The leading-order correction to the low-energy effective action is $\delta S_\mathrm{e}^{(3)}[\vec{n}]$, which can be computed as

$$\begin{aligned}\delta S_\mathrm{e}^{(3)}[\vec{n}]&=\mathcal{N}\,\mathrm{tr}(\Upsilon^a\gamma^\alpha\Upsilon^b\gamma^\beta\Upsilon^c\gamma^\gamma\Upsilon^d\Upsilon^e)\\&\quad\times\int\mathrm{d}^3x(\partial_\alpha n_a)(\partial_\beta n_b)(\partial_\sigma n_c)n_d(\delta n_\mathrm{e}),\end{aligned} \tag{A6}$$

where the integrand

$$\mathcal{N}=\int\frac{\mathrm{d}^3k}{(2\pi)^3}\frac{\Delta^5}{(\Delta^2-k^2)^4}=\frac{2\pi\mathrm{i}}{4!\,\mathrm{Area}(S^4)}. \tag{A7}$$

The trace on the right-hand side of Eq. (A6) is indeed a product of two antisymmetric tensors:

$$\mathrm{tr}(\Upsilon^a\gamma^\alpha\Upsilon^b\gamma^\beta\Upsilon^c\gamma^\tau\Upsilon^d\Upsilon^e)=8\mathrm{i}\epsilon^{\alpha\beta\tau}\epsilon^{abcde}. \tag{A8}$$

Let $\vec{n}(x,\rho)$ distort continuously such that $\vec{n}(x,0)=(n_1=1,\vec{0})$ and $\vec{n}(x,\rho=1)=\vec{n}(x)$. Thus, $\vec{n}(x)$ is defined on the four-dimensional spacetime disk D^4 with boundary $\partial D^4=S^3$. Therefore, the field $\vec{n}(x)$ defines a map from S^3 to S^4. We can introduce an auxiliary variable $\rho\in[0,1]$, and $\delta S_\mathrm{e}^{(3)}[\vec{\phi}]$ is then rewritten as

$$\begin{aligned}\delta S_\mathrm{e}^{(3)}[\vec{n}]&=8\mathrm{i}\mathcal{N}\epsilon^{\alpha\beta\sigma}\epsilon^{abcde}\int\mathrm{d}^3x\int_0^1\mathrm{d}\rho\\&\quad\times\partial_\rho[(\partial_\alpha n_a)(\partial_\beta n_b)(\partial_\tau n_c)n_d(\delta n_\mathrm{e})],\end{aligned} \tag{A9}$$

which is indeed the functional derivative of the WZW term. The field variables are defined only on the boundary, and it should be noted that the term

$$\epsilon^{\alpha\beta\sigma}\epsilon^{abcde}\int\mathrm{d}^3x\int_0^1\mathrm{d}\rho\,\partial_\alpha n_a\partial_\beta n_b\partial_\tau n_c\partial_\rho n_d\delta n_\mathrm{e} \tag{A10}$$

must vanish, since, for small changes $\vec{n}\to\vec{n}+\delta\vec{n}$, δn_e is perpendicular to n_e. Combining all these results leads to the Euclidean WZW action $S_\mathrm{WZW}^\mathrm{E}[\vec{n}]=2\pi\mathrm{i}\mathcal{S}$, with

$$\begin{aligned}\mathcal{S}&=\frac{2}{4!\,\mathrm{Area}(S^4)}\epsilon^{\alpha\beta\tau\rho}\epsilon^{abcde}\int\mathrm{d}^2x\,\mathrm{d}\tau\int_0^1\mathrm{d}\rho\\&\quad\times(\partial_\alpha n_a)(\partial_\beta n_b)(\partial_\tau n_c)(\partial_\rho n_d)n_\mathrm{e}.\end{aligned} \tag{A11}$$

Appendix B: the zero mode under twist order

We now present some results on the zero-energy modes in the Dirac Hamiltonian with static twisted backgrounds. We start with the Hamiltonian (26),

$$H=\alpha_i(-\mathrm{i}\partial_i-\gamma_5 a_{5i})+\Delta(\beta_1\cos\theta+\beta_2\sin\theta). \tag{B1}$$

The zero-energy eigenvalue equation is $H\psi_0=0$, with $\psi_0=(\psi_1,\sigma_2\psi_1^*)^\mathrm{T}$. We assume that the system is isotropic, and we set $\psi_1=[f(r,\theta),g(r,\theta)]^\mathrm{T}$. The zero-energy solutions are then determined by

$$\begin{aligned}&[\partial_+ +(a_{52}-\mathrm{i}a_{51})]f-\mathrm{i}\Delta f^*=0,\\&[\partial_- -(a_{52}+\mathrm{i}a_{51})]g+\mathrm{i}\Delta g^*=0,\end{aligned} \tag{B2}$$

where $\partial_\pm=\mathrm{e}^{\pm\mathrm{i}\theta}(\partial_r\pm\mathrm{i}\partial_\theta/2)$. For n-twisting of the scalar field, it is convenient to make the polar decomposition $\Delta=\Delta(r)\mathrm{e}^{\mathrm{i}n\theta}$, where $\Delta(r)$ vanishes at the origin and tends to a constant at infinity. The static axial gauge field a_{5i} $(i=x,y)$ integrated over a closed loop that encircles the origin yields the degree of twisting, which we can parametrize as $a_{5i}=-n\varepsilon_{ij}r_j a(r)/r^2$, $a(r\to\infty)=1/2$. The gauge field plays a role only in changing the profile of the background, but does not affect the zero-energy eigenvalue. Using polar coordinates, the eigenequations for zero energy take the form

$$\begin{aligned}&\mathrm{e}^{\mathrm{i}\theta}\left[\partial_r+\frac{\mathrm{i}\partial_\theta}{r}+\frac{na(r)}{r}\right]f-\mathrm{i}\Delta f^*=0,\\&\mathrm{e}^{-\mathrm{i}\theta}\left[\partial_r-\frac{\mathrm{i}\partial_\theta}{r}-\frac{na(r)}{r}\right]g+\mathrm{i}\Delta g^*=0.\end{aligned} \tag{B3}$$

The general ansatz for the zero-energy eigenvectors may be chosen as $f(r,\theta) = \mathrm{e}^{-\mathrm{i}\pi/4}[f_1(r)\mathrm{e}^{\mathrm{i}l_1\theta} + f_2(r)\mathrm{e}^{\mathrm{i}l_2\theta}]$, $g(r,\theta) = \mathrm{e}^{\mathrm{i}\pi/4}[g_1(r)\mathrm{e}^{\mathrm{i}m_1\theta} + g_2(r)\mathrm{e}^{\mathrm{i}m_2\theta}]$, where both $f_i(r)$ and $g_i(r)$ are real. The radial equations for $f_i(r)$ are

$$\begin{aligned}\left[\partial_r - \frac{l_1}{r} + \frac{na(r)}{r}\right] f_1 + \Delta(r) f_2 = 0,\\ \left[\partial_r - \frac{l_2}{r} + \frac{na(r)}{r}\right] f_2 + \Delta(r) f_1 = 0,\end{aligned} \tag{B4}$$

and the corresponding compatibility condition is $l_1 + l_2 = n-1$. The radial equations for $g_i(r)$ are

$$\begin{aligned}\left[\partial_r + \frac{m_1}{r} - \frac{na(r)}{r}\right] g_1 + \Delta(r) g_2 = 0,\\ \left[\partial_r + \frac{m_2}{r} - \frac{na(r)}{r}\right] g_2 + \Delta(r) g_1 = 0,\end{aligned} \tag{B5}$$

and the corresponding compatibility condition is $m_1 + m_2 = n+1$.

According to the compatibility conditions, if the total twisting of the Kekulé-VBS order is even, then all the normalized zero modes are characterized by two phases ($l_1 \neq l_2$ or $m_1 \neq m_2$); if the total twisting is odd, then one of these normalized zero modes is characterized by a single phase ($l_1 = l_2$), while the other $n-1$ normalized modes are two-phase dependent. Setting $\psi_0 = (\psi_{KA}, \psi_{KB}, \psi_{K'B}, \psi_{K'A})^{\mathrm{T}}$, the single-phase dependent wavefunction for the zero mode on sublattice A is obtained as

$$\begin{aligned}\psi_{kA} &= \mathcal{N}_A \exp\left\{-\int_0^r \left[\Delta(r) + \frac{2na(r) - (n-1)}{2r}\right] \mathrm{d}r\right\}\\ &\quad \times \exp\left\{\mathrm{i}\left[\frac{(n-1)\theta}{2} - \frac{\pi}{4}\right]\right\},\\ \psi_{k'A} &= \mathrm{i}\bar{\psi}_{kA},\end{aligned} \tag{B6}$$

where $\mathcal{N}_A$ is a normalization coefficient. Since $\Delta(r)$ and $a(r)$ vanish at small r, for the wavefunction to be normalizable, it is necessary that $n \leq -1$. Similarly, the normalizable single-phase dependent zero mode on sublattice B is obtained as

$$\begin{aligned}\psi_{kB} &= \mathcal{N}_B \exp\left\{-\int_0^r \left[\Delta(r) + \frac{(n+1) - 2na(r)}{2r}\right] \mathrm{d}r\right\}\\ &\quad \times \exp\left\{\mathrm{i}\left[\frac{(n+1)\theta}{2} + \frac{\pi}{4}\right]\right\},\\ \psi_{k'B} &= -\mathrm{i}\bar{\psi}_{kB}.\end{aligned} \tag{B7}$$

where $\mathcal{N}_B$ is a normalization coefficient. For the wavefunction at small r to be normalizable, it is necessary that $n \geq 1$. With the substitutions $\psi_{kA} \to \psi_{kB}$ and $n \to -n$, the zero-mode wavefunction on sublattice A also holds on sublattice B.

Appendix C: topological current

The Kekulé-VBS order supports vortex topological excitations. We consider the following Lagrangian with an extended order parameter $\vec{\phi} = (\Re\Delta, \Im\Delta, h)$:

$$L = \bar{\psi}\mathrm{i}\gamma^\mu(\partial_\mu - \mathrm{i}\gamma_5 a_{5\mu})\psi - \bar{\psi}\left(\sum_{k=1}^{3} \Gamma_k \phi_k\right)\psi, \tag{C1}$$

where $\Gamma_1 = \beta\beta_1 = \tau_1 \otimes \sigma_3$, $\Gamma_2 = \beta\beta_2 = \tau_2 \otimes \sigma_3$, $\Gamma_3 = \beta\mathbb{I} = \tau_0 \otimes \sigma_3$, we assume the auxiliary parameter $-\infty < h < \infty$, and the topological charge for the vortex is obtained by regularizing $h = 0$ at the end of the calculations. It should be noted that the extended order parameter breaks the chiral symmetry. Integrating over the fermion fields, we have

$$\int \mathcal{D}\bar{\psi}\mathcal{D}\psi \exp\left[-\int \mathrm{d}^3x L(\bar{\psi}, \psi, \vec{n})\right] = \mathrm{e}^{-S_{\mathrm{eff}}^{\mathrm{E}}[\vec{n}, a_{5\mu}]}, \tag{C2}$$

and the current is defined in terms of $J^\mu = \delta S_{\mathrm{eff}}^{\mathrm{E}}/\delta a_{5\mu}|_{a_{5\mu}=0}$. Again, using the gradient expansion,[45] we have

$$J^\mu = \frac{\delta S_{\mathrm{eff}}^{\mathrm{E}}}{\delta a_{5\mu}} = -\mathrm{Tr}\{\gamma_5\gamma^\mu \mathcal{G}_0^{-1}[\mathcal{G}_0^{-1}(\mathcal{G}_0^{-1})^\dagger]^{-1}\}, \tag{C3}$$

where $\mathcal{G}_0^{-1} = \mathrm{i}\gamma^\mu\partial_\mu - \Gamma_k\phi_k$. The gradient expansion yields

$$J^\mu = -\sum_{l=0}^{\infty} \mathrm{Tr}\left[\gamma_5\gamma^\mu \frac{\mathrm{i}\gamma^\nu\partial_\nu - \Gamma_k\phi_k}{-\partial^2 + \phi^2}\left(\frac{-\mathrm{i}\Gamma_k\gamma^\lambda\partial_\lambda\phi_k}{-\partial^2+\phi^2}\right)^l\right]. \tag{C4}$$

It is easily checked that both the $l = 0$ and $l = 1$ terms vanish and the dominant term is

$$\begin{aligned}J^\mu &= \mathrm{Tr}\left[\gamma_5\gamma^\mu \frac{\Gamma_k\phi_k}{-\partial^2+\phi^2}\left(\frac{-\mathrm{i}\gamma^\lambda\Gamma_k\partial_\lambda\phi_k}{-\partial^2+\phi^2}\right)^2\right]\\ &= \int \frac{\mathrm{d}^3k}{(k^2+\phi^2)^3}\mathrm{Tr}(\gamma^\mu\gamma^\nu\gamma^\lambda\Gamma_5\Gamma_a\Gamma_b\Gamma_c)\,\phi^a\partial_\nu\phi^b\partial_\lambda\phi^c\\ &= -\frac{1}{8\pi\phi^3}\epsilon^{\mu\nu\lambda}\epsilon^{abc}\phi^a\partial_\nu\phi^b\partial_\lambda\phi^c,\end{aligned} \tag{C5}$$

where $k^2 = k_0^2 - \boldsymbol{k}^2$, and the topological charge is defined as $q = \int \mathrm{d}^2x J^0$.

Acknowledgment

We acknowledge helpful communications with Martin Hohenadler.

References

[1] Sachdev S 2011 *Quantum Phase Transitions* (2nd Edn) (Cambridge: Cambridge University Press)
[2] Read N and Green D 2000 *Phys. Rev. B* **61** 10267
[3] Li Z X, Jiang Y F, Jian S K and Hong Y 2017 *Nat. Commun.* **8** 314
[4] Jian S K and Yao H 2017 *Phys. Rev. B* **96** 195162
[5] Jian S K and Yao H 2017 *Phys. Rev. B* **96** 155112
[6] You Y Z, He Y C, Xu C and Vishwanath A 2018 *Phys. Rev. X* **8** 011026
[7] Classen L, Herbut I F and Scherer M M 2017 arXiv:1705.08973v2
[8] Scherer M M and Herbut I F 2016 *Phys. Rev. B* **94** 205136
[9] Roy Bitan, Juricic V and Herbut I F 2013 *Phys. Rev. B* **87** 041401(R)
[10] Senthil T, *et al.* 2004 *Science* **303** 1490
[11] Qi X L and Zhang S C 2011 *Rev. Mod. Phys.* **83** 1057
[12] Hasan M Z and Kane C L 2011 *Rev. Mod. Phys.* **82** 3054
[13] Haldane F D M 1988 *Phys. Rev. Lett.* **61** 2015
[14] Zhang J, Zhao B, Zhou T and Yang Z 2016 *Chin. Phys. B* **25** 117308

[15] Burkov A A, Hook M M and Balents L 2011 *Phys. Rev. B* **84** 235126
[16] Xiang H J 2017 *Chin. Phys. Lett.* **34** 057302
[17] Fu L and Kane C L 2008 *Phys. Rev. Lett.* **100** 096407
[18] Wu B, Song J, Zhou J and Jiang H 2016 *Chin. Phys. B* **25** 117311
[19] Wu W, Rachel S, Liu W M and Hur K L 2012 *Phys. Rev. B* **85** 205102
[20] Wu W, Chen Y H, Tao H S, Tong N H and Liu W M 2010 *Phys. Rev. B* **82** 245102
[21] Zhou Z, Da W, Meng Z Y, Wang Y and Wu C 2016 *Phys. Rev. B* **93** 245157
[22] Zhou Z, Da W, Wu C and Wang Y 2017 *Phys. Rev. B* **95** 085128
[23] Otsuka Y, Yunoki S and Sorella S 2017 *Phys. Rev. X* **6** 011029
[24] Li Z X, Jiang Y F and Yao H 2015 *New J. Phys.* **17** 085003
[25] Capello M, Becca F, Yunoki S and Sorella S 2006 *Phys. Rev. B* **73** 245116
[26] Meng Z Y, Lang T C, Wessel S, Assaad F F and Muramatsu A 2010 *Nature* **464** 847
[27] Griset C and Xu C 2012 *Phys. Rev. B* **85** 045123
[28] Moon E G and Xu C 2012 *Phys. Rev. B* **86** 214414
[29] Sato T, Hohenadler M and Fakher F A 2017 *Phys. Rev. Lett.* **119** 197203
[30] Herbut I F 2006 *Phys. Rev. Lett.* **97** 146401
[31] Herbut I F, Juricic V and Roy B 2009 *Phys. Rev. B* **79** 085116
[32] Herbut I F, Juricic V and Vafek O 2009 *Phys. Rev. B* **80** 075432
[33] Toldin F P, Martin H, Fakher F A and Herbut I F 2015 *Phys. Rev. B* **91** 165108
[34] Fakher F A and Herbut I F 2013 *Phys. Rev. X* **3** 031010
[35] Ghaemi P and Ryu S 2012 *Phys. Rev. B* **85** 075111
[36] Ryu S, Mudry C, Hou C Y and Chamon C 2009 *Phys. Rev. B* **80** 205319
[37] Hosur P, Ryu S and Vishwanath A 2010 *Phys. Rev. B* **81** 045120
[38] Matthias V, Ying Z and Subir S 2000 *Phys. Rev. B* **62** 10
[39] Subir S 2000 *Science* **288** 475
[40] Xu C and Subir S 2009 *Phys. Rev. B* **79** 064405
[41] Moon E G 2016 *Sci. Rep.* **6** 31051
[42] Tanaka A 2011 *J. Phys.: Conf. Ser.* **320** 012020
[43] Tanaka A and Hu X 2005 *Phy. Rev. Lett.* **95** 036402
[44] Grover T and Senthil T 2008 *Phys. Rev. Lett.* **100** 156804
[45] Abanov A G and Wiegmann P B 2000 *Nucl. Phys. B* **570** 685
[46] Senthil T and Matthew P A F 2006 *Phys. Rev. B* **74** 064405
[47] Xu C 2012 *Int. J. Mod. Phys. B* **26** 1230007
[48] Balents L, Fisher M P A and Nayak C 1999 *Phys. Rev. B* **60** 1654
[49] Kou S P, Qi X L and Weng Z Y 2005 *Phys. Rev. B* **71** 235102
[50] Wang Q H 2003 *Chin. Phys. Lett.* **20** 1582
[51] Wang Q H 2004 *Phys. Rev. Lett.* **92** 057003
[52] Jian S K and Yao H 2018 arXiv:1805.12299v1
[53] Hou C Y, Chamon C and Mudry C 2007 *Phys. Rev. Lett.* **98** 186809
[54] Ran Y, Vishwanath A and Lee D H 2008 *Phys. Rev. Lett.* **101** 086801
[55] Qi X L and Zhang S C 2008 *Phys. Rev. Lett.* **101** 086802
[56] Jackiw R and Rossi P 1981 *Nucl. Phys. B* **190** 681
[57] Weinberg E J 1981 *Phys. Rev. D* **24** 2669
[58] Qin Y Q, He Y Y, You Y Z, Lu Z Y, Sen A, Sandvik A W, Xu C and Meng Z Y 2017 *Phys. Rev. X* **7** 031052
[59] Wang C, Nahum A, Metlitski M A, Xu C and Senthil T 2017 *Phys. Rev. X* **7** 031051
[60] Janssen L and He Y C 2017 *Phys. Rev. B* **96** 205113