Weyl semimetal and nonassociative Nambu geometry

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Topological materials are characterized by an electronic band structure with nontrivial topological properties. In this paper we introduce a basis of operators for the linear space of operators spanned by charge-neutral fermion bilinears. These band-projected density operators are constructed using directly the eigenfunctions of the electronic energy band structure and there is no need to assume a flat Berry curvature. As a result, our set of operators has a wider range of validity and is sensitive to physical phenomena which are not detectable in the flat-curvature limit. In particular, we show that the Berry monopole configuration of a Weyl semimetal give rises to a nonvanishing Jacobiator for these band-projected density operators, implying the emergence of nonassociativity at the location of the Weyl nodes. The resulting nonassociativity observes the fundamental identity, the defining property of the Nambu bracket, and so one may call this a nonassociative Nambu geometry. We also derive the corresponding uncertainty principle.

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I. INTRODUCTION

Topological material is one of the recent hot topics of research in condensed matter physics. These are novel electronic states of matter with properties supported by topology. Topological material has not only overturned the traditional Landau paradigm on the classification of condensed matter states; it has also many remarkable properties that are not only interesting theoretically, but has also important potential practical applications, such as topological quantum computing [1].

A topological insulator (TI) is the simplest form of topological material. Different from an ordinary insulator, a TI is conducting at the boundary due to the existence of gapless chiral states at the surface, which in turn is a result of the nontrivial momentum space topology of the bulk band structure. As long as the band gap is not closed, the topological ground state is robust against small perturbations and the surface states are protected. The Chern insulator (CI) is the most primitive example of a topological insulator. As a two-dimensional system, it has a band structure which is characterized by the first Chern number of the Berry connection associated with the Bloch waves, and exhibits a quantized Hall conductance even without an external magnetic field [2], generalizing the original integer quantum Hall effect (IQHE) [3] for the filled Landau levels [4]. In the presence of time-reversal symmetry (TRS), the first Chern numbers and the Hall conductivity must vanish. However the spin-orbit interaction allows a different topological class of insulating band structures, giving rise to the $\mathbb{Z}_2$ topological insulator in two and three dimensions [5–8], leading to successful prediction and experimental observation of these phases of materials [9–14].

A slightly more complicated and also much more interesting topological material is the fractional Chern insulator (FCI), where the topological bands are partially filled. The best known example is the the fractional quantum Hall effect (FQHE) [15], a strongly correlated phenomena which arises from the huge degeneracy within the Landau levels for particles in a magnetic field. Here a very useful observable is the density operator projected to the lowest Landau level. These operators were introduced originally by Girvin, Macdonald, and Platzman (GMP) [16], and were found to obey a W_∞ Lie algebra [17], which reflects the area-preserving incompressible nature of the Laughlin wave functions of the FQHE [18]. Inspired by the success of the algebraic approach of GMP to the problems of IQHE and FQHE, Haldane proposed recently a geometrical description of the FQHE based on the algebra of these projected density operators [19]. More recently, a specific noncommutative geometry for the band-projected density operators was identified by Parameswaran, Roy, and Sondhi [20] for general two-dimensional CIs and FCIs. See also [21–24] for related algebraic approaches. A reformulation of the Hamiltonian theory of the FQHE was introduced in [25,26]. Our work is motivated by these studies.

The noncommutative geometry identified by [20] generalizes the well known noncommutative geometry obeyed by the guiding center of the Landau level electron $[X,Y] = il_B^2$, where $l_B = \sqrt{\hbar/eB}$ is the magnetic length. In the limit of long wavelength and flat Berry curvature, it coincides with the noncommutative geometry of GMP. The noncommutative geometry is expected to be useful since in the limit the band structure admits a large band gap compared to the interaction strength, which is relevant for the studies of the FQHE; it makes sense to project the problem to the lowest filled band where the major effects of the interaction take place. Due to the universality of the identified noncommutative geometry, Parameswaran, Roy, and Sondhi also proposed that the band noncommutative geometry could be useful to the study of the FQHE in FCIs in a similar way. The noncommutative geometry of topological insulators was then further studied in the three- and the higher-dimensional case [27–33]. In particular, an interesting 3-bracket utilizing the complete antisymmetrizer has been constructed for the differentiated projected density operators in 3 dimensions in [27].

We remark that the above mentioned noncommutative geometries were obtained as a property of the electronic band. They are purely kinematical and independent of interaction. Furthermore it does not matter whether the material is topological or not; the noncommutative geometry takes on the same universal form with the dependence on the materials entering only through the band's Berry connection. This motivates us to ask whether there exists a more refined characterization of topological materials that is intrinsic to the nontrivial topology. We find in this paper that the Weyl semimetal is characterized by a nonassociative geometry (28) of the projected density operators.

The Weyl semimetal (WSM) is an interesting class of topological materials that lives in 3 dimensions. Unlike a topological insulator, the valence band and the conduction band of a WSM touch at isolated points in the momentum space. The nodal point is called a Weyl node since the nearby band structure is described by the Hamiltonian of a massless Weyl fermion, and, depending on the chirality of the node, the associated Berry connection describes a monopole or antimonopole in the 3-dimensional momentum space. Weyl nodes are topological objects.

The only way for the Weyl nodes to disappear is to annihilate them in pairs. In fact, the theorem of Nielsen and Ninomiya states that Weyl nodes always come in pairs of opposite chirality [34]. Therefore to obtain a stable WSM, its Weyl nodes need to stay separated in momentum space in order to prevent them from annihilation. This can be achieved when either TR or inversion symmetry is broken. In the presence of both TR and inversion symmetry, the touched band must be doubly degenerate and one obtain a Dirac fermion spectrum near the nodal points, resulting in the so called Dirac semimetal (DSM).

As a result of the topologically nontrivial band structure, like any other topological materials, the WSM is also endowed with topologically protected surface states, the Fermi arcs [35]. One particularly illuminating way [36] to understand the origin of the Fermi arcs is to consider a slicing of the Brillouin zone (BZ). Each momentum space slice of the WSM which does not contain the Weyl nodes is a Chern insulator whose Chern number changes by ± 1 as one sweeps past a Weyl node. Thus if the slices in between the nodes have a unit Chern number, i.e., these slices are nontrivial CIs, then the Fermi arcs are simply the edge states of these CIs. The simple connection between Weyl semimetal and Chern insulator illustrated in this picture also suggests that some of what we know about two-dimensional CIs could be and should be generalized to the 3-dimensional case. This is another motivation of this paper.

The planning of this paper is as follows. In Sec. II A, we first review the noncommutative geometry for band-projected density operators. We also generalize the result to more general band-projected operators. In Sec. II B, we compute the Jacobiator for the band-projected operators and find that it is nonzero in the presence of a monopole. This is the case as in the Weyl semimetal. We also explain the origin of the nonassociativity. In Sec. II C, we show that the obtained Jacobiator satisfies the fundamental identity, the defining property of the Nambu bracket [37]. As a result, we call this the *nonassociative Nambu geometry*. In Sec. III, we consider the uncertainty principle of the nonvanishing Jacobiator. Just as a nonvanishing commutator leads to the Heisenberg uncertainty principle that involves a product of the uncertainties of the operators appearing in the commutator, we show that a nonvanishing Jacobiator leads to similar uncertainty principles that involve a product of the uncertainties of the operators appearing in the Jacobiator.

II. QUANTUM GEOMETRY OF TOPOLOGICAL BAND

In the band theory of crystal structure, the motion of a single electron can be approximated by treating the whole lattice of ions and other electrons as a static background. We consider an insulator with N bands. The single-particle Hamiltonian takes the form

$$H_0 = \sum_{a,b,\mathbf{k}} c^\dagger_{\mathbf{k},a} h_{ab}(\mathbf{k}) c_{\mathbf{k},b}, \tag{1}$$

where $a,b = 1,\ldots,N$ label the states in the unit cell, $\mathbf{k} = (k_1,\ldots,k_D)$ is the single-particle momentum restricted to the first Brillouin zone, and D is the (spatial) dimension of the material. The Hamiltonian can be diagonalized straightforwardly by considering the eigenvalue problem

$$\sum_b h_{ab}(\mathbf{k}) u^\alpha_b(\mathbf{k}) = E_\alpha(\mathbf{k}) u^\alpha_a(\mathbf{k}), \tag{2}$$

where $\alpha = 1,\ldots,N$ labels the band energy $E_\alpha(\mathbf{k})$. Adopting the orthonormality condition for the eigenfunctions

$$\sum_a u^\alpha_a(\mathbf{k})^* u^\beta_a(\mathbf{k}) = \delta^{\alpha\beta}, \tag{3}$$

the orbital creation operator

$$\gamma^{\alpha\dagger}_{\mathbf{k}} := \sum_a u^\alpha_a(\mathbf{k}) c^\dagger_{\mathbf{k},a} \tag{4}$$

obeys

$$\left[\gamma^{\alpha\dagger}_{\mathbf{k}}, \gamma^\beta_{\mathbf{q}}\right]_+ = \delta_{\mathbf{k},\mathbf{q}} \delta^{\alpha\beta}, \tag{5}$$

and the Hamiltonian can be written in the diagonalized form

$$H_0 = \sum_{\mathbf{k},\alpha} E_\alpha(\mathbf{k}) \gamma^{\alpha\dagger}_{\mathbf{k}} \gamma^\alpha_{\mathbf{k}} \tag{6}$$

with the eigenstates

$$|\mathbf{k},\alpha\rangle = \gamma^\dagger_{\mathbf{k},\alpha}|0\rangle. \tag{7}$$

Despite the simple appearance of (6), the information encoded in the eigenfunctions $u^\alpha_b(\mathbf{k})$ is not lost. One of the remarkable features of the energy band structure is that it is naturally equipped with a Berry connection. For a given band α, the Berry connection is defined by

$$A^\alpha_j(\mathbf{k}) = i \sum_{b=1}^N u^\alpha_b(\mathbf{k})^* \frac{\partial}{\partial k_j} u^\alpha_b(\mathbf{k}), \quad j = 1,\ldots,D. \tag{8}$$

The definition can be straightforwardly generalized to a non-Abelian Berry connection involving an arbitrary number of bands. In the standard application, the Berry connection is kinematical. Taking into account the fluctuation of the crystal ions, one may wonder whether a kinetic term would be induced as in induced gravity [38].

A. Noncommutative geometry for band-projected operators

Making use of the projection operator $P_\alpha = \sum_{\mathbf{k}} |\mathbf{k},\alpha\rangle\langle\mathbf{k},\alpha|$, one can project the density operator

$\rho_{\mathbf{q}} = e^{i\mathbf{q}\cdot\mathbf{r}}$ onto the band α. In momentum space, the projected density operator takes the form [20]

$$\hat{\rho}_{\mathbf{q},\alpha} := P_\alpha \rho_{\mathbf{q}} P_\alpha = \sum_{\mathbf{k},b} u_b^{\alpha *}\Big(\mathbf{k}+\frac{\mathbf{q}}{2}\Big) u_b^{\alpha}\Big(\mathbf{k}-\frac{\mathbf{q}}{2}\Big) \times \gamma^{\alpha\,\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}} \gamma^{\alpha}_{\mathbf{k}-\frac{\mathbf{q}}{2}}. \tag{9}$$

It is

$$\hat{\rho}^{\dagger}_{\mathbf{q},\alpha} = \hat{\rho}_{-\mathbf{q},\alpha}. \tag{10}$$

In the following we will focus on a single band and so we will skip the subscript α and simply write $\hat{\rho}_{\mathbf{q},\alpha}$ as $\hat{\rho}_{\mathbf{q}}$. In the paper [20], it was found that the density operator at different momentum obeys, in the leading order of small momentum, the commutator relation:

$$[\hat{\rho}_{\mathbf{q}_1}, \hat{\rho}_{\mathbf{q}_2}] = i q_1^i q_2^j \sum_{\mathbf{k},b} F_{ij}(\mathbf{k}) u_b^{\alpha *}\Big(\mathbf{k}+\frac{\boldsymbol{q}}{2}\Big) u_b^{\alpha}\Big(\mathbf{k}-\frac{\boldsymbol{q}}{2}\Big) \times \gamma^{\alpha\,\dagger}_{\mathbf{k}+\frac{\boldsymbol{q}}{2}} \gamma^{\alpha}_{\mathbf{k}-\frac{\boldsymbol{q}}{2}}, \tag{11}$$

where

$$F_{ij}(\mathbf{k}) := \partial_i A_j(\mathbf{k}) - \partial_j A_i(\mathbf{k}) \tag{12}$$

is the curvature of the Berry connection, and $\boldsymbol{q} := \sum_n \mathbf{q}_n = \mathbf{q}_1 + \mathbf{q}_2$ is the sum of the momentum of the operators on the right-hand side of (11). The noncommutative relation (11) is interesting. It is an universal property of band insulators. It takes the same form even when the material is nontopological with vanishing Chern numbers. In the literature sometimes it is considered the situation of having a Berry curvature slowly varying over the BZ. In this case, (11) takes the approximate form

$$[\hat{\rho}_{\mathbf{q}_1}, \hat{\rho}_{\mathbf{q}_2}] \approx i q_1^i q_2^j \bar{F}_{ij}\ \hat{\rho}_{\mathbf{q}_1+\mathbf{q}_2}, \tag{13}$$

where $\bar{F}_{ij}$ is the mean value of the Berry curvature over the BZ. The result (13) is now topological: it is nontrivial only when the Chern number is nonvanishing. In this paper, we will be interested in the general behavior of the Berry connection without making any assumption that it is slowly varying. In particular, our main results (22), (25) about the Jacobiator are nontrivial only in the presence of monopoles and nontrivial topology. This is in contrast with the noncommutative geometry (11) which can be nontrivial even in the absence of nontrivial topology.

It is instructive to generalize the result (11) for the commutator of two projected density operators. In general for any arbitrary function $f(\mathbf{k})$ defined on the BZ and momentum $\mathbf{q}$, one can introduce the band-projected operator

$$\mathcal{O}(f,\mathbf{q}) = \sum_{\mathbf{k},b} f(\mathbf{k}) u_b^{\alpha *}\Big(\mathbf{k}+\frac{\mathbf{q}}{2}\Big) u_b^{\alpha}\Big(\mathbf{k}-\frac{\mathbf{q}}{2}\Big) \times \gamma^{\alpha\,\dagger}_{\mathbf{k}+\frac{\mathbf{q}}{2}} \gamma^{\alpha}_{\mathbf{k}-\frac{\mathbf{q}}{2}} \tag{14}$$

in association with the band α. As explained above, we will ignore the band index. Note that since $\mathcal{O}$ depends linearly on its first argument, it is obvious that

$$\mathcal{O}(f,\mathbf{q}) + \mathcal{O}(g,\mathbf{q}) = \mathcal{O}(f+g,\mathbf{q}). \tag{15}$$

It is obvious that the set of operators (14) forms an overcomplete basis for the linear space of operators spanned by charge-neutral fermion bilinears. The operators (14) provide a generalization of the projected density operator and can be used to describe more complicated interaction than the density-density type. It is natural to ask whether the set $\mathscr{A}$ of operators $\mathcal{O}$ for all functions f defined on the BZ forms a Lie algebra, and if so, of what kind.

Therefore, let us consider the commutator. It is clear from the definition (14) of the operator that the commutator of these operators gives something that is bilinear in the orbital creation operator

$$[\mathcal{O}(f_1,\mathbf{q}_1), \mathcal{O}(f_2,\mathbf{q}_2)] = \sum_{\mathbf{k},b,c} K_{bc}(\mathbf{k},\mathbf{q}_1,\mathbf{q}_2) \times \gamma^{\alpha\,\dagger}_{\mathbf{k}_+} \gamma^{\alpha}_{\mathbf{k}_-}, \tag{16}$$

where $\mathbf{k}_\pm := \mathbf{k} \pm \frac{\boldsymbol{q}}{2}$, $\boldsymbol{q} := \mathbf{q}_1 + \mathbf{q}_2$, and K is some kernel depending on b,c and the momentum $\mathbf{q}_1,\mathbf{q}_2$, and $\mathbf{k}$. It is given by

$$\begin{aligned} K_{bc}(\mathbf{k},\mathbf{q}_1,\mathbf{q}_2) = {}& f_1\Big(\mathbf{k}-\frac{\mathbf{q}_2}{2}\Big) f_2\Big(\mathbf{k}+\frac{\mathbf{q}_1}{2}\Big) \\ & \times u_b^*(\mathbf{k}_+ - \mathbf{q}_2) u_b(\mathbf{k}_-) u_c^*(\mathbf{k}_+) u_c(\mathbf{k}_- + \mathbf{q}_1) \\ & - f_1\Big(\mathbf{k}+\frac{\mathbf{q}_2}{2}\Big) f_2\Big(\mathbf{k}-\frac{\mathbf{q}_1}{2}\Big) u_b^*(\mathbf{k}_+) u_b \\ & \times (\mathbf{k}_- + \mathbf{q}_2) u_c^*(\mathbf{k}_+ - \mathbf{q}_1) u_c(\mathbf{k}_-). \end{aligned} \tag{17}$$

In general K_{bc} is not diagonal and thus the commutator of $\mathcal{O}$'s does not close back to $\mathcal{O}$. However, in the approximation of small momentum $\mathbf{q}_1,\mathbf{q}_2$, one can expand K. It turns out that the leading term in the approximation of small momentum is diagonal in b,c and takes the simple form

$$\begin{aligned} & K_{bc}(\mathbf{k},\mathbf{q}_1,\mathbf{q}_2) \\ & = \delta_{bc}\ \big(i q_1^i q_2^j (F_{ij} f_1 f_2)(\mathbf{k}) + q_1^i (f_1 \partial_i f_2)(\mathbf{k}) \\ & \quad - q_2^i (f_2 \partial_i f_1)(\mathbf{k})\big) u_b^{\alpha *}\Big(\mathbf{k}+\frac{\boldsymbol{q}}{2}\Big) u_b^{\alpha}\Big(\mathbf{k}-\frac{\boldsymbol{q}}{2}\Big) + \cdots, \end{aligned} \tag{18}$$

where $\cdots$ denotes terms that are higher order in the momentum $\mathbf{q}_1$ or $\mathbf{q}_2$. As a result, in the leading order of small momentum, the operators $\mathcal{O}$ obey the operator relation (19),

$$[\mathcal{O}(f_1,\mathbf{q}_1), \mathcal{O}(f_2,\mathbf{q}_2)] = \mathcal{O}(\{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2)\}, \mathbf{q}_1+\mathbf{q}_2), \tag{19}$$

where the 2-bracket $\{,\}$ is defined by

$$\begin{aligned} \{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2)\} := {}& (i q_1^i q_2^j (F_{ij} f_1 f_2) + q_1^i (f_1 \partial_i f_2) \\ & - q_2^i (f_2 \partial_i f_1), \mathbf{q}_1 + \mathbf{q}_2). \end{aligned} \tag{20}$$

The bracket $\{,\}$ is defined for any pair of objects $(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2)$, where the f_n's are functions defined on the BZ and the $\mathbf{q}_n$'s are momenta restricted to the BZ. Note that the momenta $\mathbf{q}_1,\mathbf{q}_2$ enter linearly in the 2-bracket $\{,\}$. Effectively, we have shown that, in the leading order of small momentum, the set $\mathscr{A}$ can be endorsed with a commutator, with respect to which it becomes a closed algebra. Furthermore, the commutation relation of $\mathcal{O}$ induces a 2-bracket $\{,\}$ on the pair of objects $(f,\mathbf{q})$.

We remark that a different set of fermion bilinear operators has been introduced before [23,24,26]. These operators form a Lie algebra, and, for even dimensions, constitute a complete basis [24]. In contrast to these operators, which were suitably defined in the limit of a flat Berry curvature, our operators (14) are constructed directly using the eigenfunctions of the electronic energy band and there is no need to assume a flat Berry curvature. Because of this, our set of operators has a wider range of validity and is sensitive to physical phenomena which are not detectable in the flat-curvature limit. In particular, our set of operators could provide support to a kind of nonassociative geometry which occurs in the presence of monopoles. This is another main result of this paper.

B. Nonassociative geometry and monopoles

To decide whether it is a Lie algebra, we need to check the Jacobi identity. After a long but straightforward computation, we find

$$\{\{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2)\},(f_3,\mathbf{q}_3)\} + \text{cyclic} = \left(-if_1f_2f_3 \sum_{i,j,k=1}^{D} q_1^i q_2^j q_3^k(\partial_i F_{jk} + \text{cyclic}), \boldsymbol{q}\right). \quad (21)$$

Here $\boldsymbol{q} := \sum_n \mathbf{q}_n = \mathbf{q}_1 + \mathbf{q}_2 + \mathbf{q}_3$ is the sum of momenta of the operators on the left-hand side of Eq. (21). We note that in principle the left-hand side of (21) contains terms of the form $fgq\partial_i h$ with one derivative acting on f,g, or h, and terms of the form $f_1f_2\partial_i\partial_j f_3$ and $f_1\partial_i f_2\partial_j f_3$ with two derivatives acting on the f_n's. However all these terms get canceled with each other and in the end only the nonderivative term $f_1f_2f_3$ is left over. Hence the result (21) is exact and there is no need to make any assumption of small momentum.

It follows from (21) that the Jacobiator for the operators $\mathcal{O}$ takes the simple form

$$[\mathcal{O}(f_1,\mathbf{q}_1),\mathcal{O}(f_2,\mathbf{q}_2),\mathcal{O}(f_3,\mathbf{q}_3)] = -if_1f_2f_3 \sum_{i,j,k=1}^{D} q_1^i q_2^j q_3^k \ \mathcal{O}(\partial_i F_{jk} + \text{cyclic}, \boldsymbol{q}) \quad (22)$$

in the leading order of small momentum. Here the Jacobiator for any three operators A,B,C is defined as

$$[A,B,C] := [[A,B],C] + [[B,C],A] + [[C,A],B]. \quad (23)$$

For 3 dimensions, we have

$$\{\{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2)\},(f_3,\mathbf{q}_3)\} + \text{cyclic} = (-if_1f_2f_3\,(\mathbf{q}_1\times\mathbf{q}_2)\cdot\mathbf{q}_3\ \nabla\cdot\mathbf{B},\ \boldsymbol{q}) \quad (24)$$

and

$$[\mathcal{O}(f_1,\mathbf{q}_1),\mathcal{O}(f_2,\mathbf{q}_2),\mathcal{O}(f_3,\mathbf{q}_3)] = -if_1f_2f_3\,(\mathbf{q}_1\times\mathbf{q}_2)\cdot\mathbf{q}_3\ \mathcal{O}(\nabla\cdot\mathbf{B},\ \boldsymbol{q}) \quad (25)$$

in the leading order of small momentum. We note that the right-hand sides of (21), (22), (24), and (25) are zero for smooth configurations of the Berry connection since the Berry curvature F_{ij} is a total derivative. In this case the 2-bracket $\{,\}$ defines a Lie bracket on $\mathscr{A}$ and the operator product between the operators $\mathcal{O}$ is associative. However in the presence of a monopole, which is characteristic of a topological insulator, the Jacobi identity (21) is violated and the 2-bracket $\{,\}$ does not define a Lie bracket. Correspondingly the operator algebra $\mathscr{A}$ is nonassociative.

The projected density corresponds to the simplest case of a constant function $f = 1$,

$$\hat{\rho}_{\mathbf{q}} = \mathcal{O}(1,\mathbf{q}), \quad (26)$$

and the result (11) follows immediately from the 2-bracket (20) that

$$\{(1,\mathbf{q}_1),(1,\mathbf{q}_2)\} = iq_1^i q_2^j F_{ij}. \quad (27)$$

As for the Jacobiator, we have for 3 dimensions the result

$$[\hat{\rho}_{\mathbf{q}_1},\hat{\rho}_{\mathbf{q}_2},\hat{\rho}_{\mathbf{q}_3}] = -i(\mathbf{q}_1\times\mathbf{q}_2)\cdot\mathbf{q}_3 \sum_{\mathbf{k},b} \nabla\cdot\mathbf{B}(\mathbf{k})u_b^{\alpha *}\left(\mathbf{k}+\frac{\boldsymbol{q}}{2}\right)u_b^{\alpha} \times \left(\mathbf{k}-\frac{\boldsymbol{q}}{2}\right) \times \gamma_{\mathbf{k}+\frac{\boldsymbol{q}}{2}}^{\alpha\,\dagger}\gamma_{\mathbf{k}-\frac{\boldsymbol{q}}{2}}^{\alpha}. \quad (28)$$

We comment that in contrast to the commutation relation (11) which takes the same form universal to all energy band, the violation of nonassociativity spotted by the Jacobiator (28) is an intrinsic characterization of a topological Weyl semimetal.

The emergence of nonassociativity is not a new phenomenon in physics. As far as we know, the Jacobiator first appeared in the literature of particle physics and quantum field theory in the computation of the space components of current in the quark model [39,40]. Later, a proper understanding of the Jacobiator in terms of the 3-cocycle of an associated (nonassociative) group transformation was developed in [41–44]. Moreover, as an example, the quantization of a charged particle in a magnetic monopole is shown to give rise to a nonvanishing Jacobiator. Let us recall briefly this result. Consider a charged particle in the presence of an external magnetic field $\mathbf{B}$ in 3 dimensions. A gauge-invariant canonical momentum does not exist. Instead the velocity operator $v_i = (p_i + eA_i)/m$ is gauge invariant. The velocities do not commute,

$$[v_i,v_j] = i\frac{e\hbar}{m^2}\epsilon_{ijk}B_k, \quad (29)$$

and have the Jacobiator

$$[v_3,[v_1,v_2]] + (123)\text{ cyclic} = \frac{e\hbar^2}{m^3}\nabla\cdot\mathbf{B}, \quad (30)$$

which is nonvanishing in the presence of a magnetic monopole, $\nabla\cdot\mathbf{B} = 4\pi g \neq 0$. The presence of nonassociativity in the operator algebra means that the velocity operators are not globally defined. This is becasue the vector potentials are not globally defined in the presence of a monopole, in which case we can either use a singular description involving a Dirac string, or equivalently, use the Wu-Yang description which employs two patches of potential related by a gauge transformation. At the level of a gauge bundle, the monopole charge g must satisfy the Dirac quantization condition $eg = \frac{\hbar}{2}\mathbb{Z}$. The same condition guarantees that translations commute and a proper quantum mechanical formalism exists [41–44].

Our consideration and analysis has in fact been motivated by the knowledge of this simple system. In particular the striking similarity of (11) with (29) has leaded us to suspect that the Jacobiator of the projected density operators will be proportional to $\nabla\cdot\mathbf{B}$ and this is indeed the case as we obtained in (28). In our case, however, the breakdown of the associativity is more basic. It is due to the merging of the bands at the Weyl node, which results in a change of the degeneracy of the energy levels. Recall how the projected density operator acts on the states (7)

$$\hat{\rho}_{\mathbf{q}}|\mathbf{k},\alpha\rangle = e^{i\int_{\mathbf{k}}^{\mathbf{k}+\mathbf{q}} d\mathbf{k}'\cdot\mathbf{A}(\mathbf{k}')}|\mathbf{k}+\mathbf{q},\alpha\rangle \tag{31}$$

in the long-wavelength limit. The occurrence of degeneracy leads to a Berry monopole configuration [45]. This in principle is bad for (31) since the corresponding Berry connection contains a Dirac string singularity. However it is well known that if the Dirac quantization condition is satisfied, then the Dirac string singularity becomes a gauge artifact, and hence the representation (31) is well defined. Nevertheless the presence of the monopole is physical and we find that its singular nature is felt through a certain successive action, the Jacobiator, of the band-projected operators.

C. Fundamental identity and Nambu geometry

Next we would like to characterize the kind of nonassociative geometry (25) we are having here. In general, given an algebra with a binary product $\circ$, one can introduce the associator defined by

$$\delta(A,B,C) := (A\circ B)\circ C - A\circ(B\circ C) \tag{32}$$

to characterize the nonassociativity of the algebra. The associator is related to the Jacobiator as

$$\begin{aligned}[A,B,C] :&= \delta(A,B,C)+\delta(B,C,A)+\delta(C,A,B)\\ &\quad -\delta(B,A,C)-\delta(C,B,A)-\delta(A,C,B).\end{aligned} \tag{33}$$

As we have just demonstrated, the algebra $\mathscr{A}$ of operators $\mathcal{O}$ is nonassociative in general. It is interesting to characterize the type of the nonassociative geometry. A first guess which comes to the mind is the Malcev algebra that has also appeared in some studies in string theory [46]. In general, a Malcev algebra $\mathscr{A}$ is an algebra equipped with an antisymmetric product $\circ$,

$$x_1\circ x_2 = -x_2\circ x_1, \tag{34}$$

in which the Malcev identity

$$\begin{aligned}&(x_1\circ x_2)\circ(x_1\circ x_3)\\ &\quad = \{[(x_1\circ x_2)\circ x_3]\circ x_1\} + \{[(x_2\circ x_3)\circ x_1]\circ x_1\}\\ &\qquad + \{[(x_3\circ x_1)\circ x_1]\circ x_2\}\end{aligned} \tag{35}$$

is satisfied for any $x_1,x_2,x_3 \in \mathscr{A}$.

In our case we can define an antisymmetric product from the commutator

$$x_1\circ x_2 := [x_1,x_2]. \tag{36}$$

Then, in terms of the Jacobiator, the Malcev identity reads

$$[[x_1,x_2,x_3],x_1] = [x_1,x_2,[x_3,x_1]]. \tag{37}$$

Taking $x_n = \mathcal{O}(f_n,\mathbf{q}_n)$, the operator relation is translated to the following statement on the 2-bracket:

$$\begin{aligned}&\{\{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2),(f_3,\mathbf{q}_3)\},(f_1,\mathbf{q}_1)\}\\ &\quad = \{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2),\{(f_3,\mathbf{q}_3),(f_1,\mathbf{q}_1)\}\},\end{aligned} \tag{38}$$

where

$$\begin{aligned}\{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2),(f_3,\mathbf{q}_3)\} :&= \{\{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2)\},(f_3,\mathbf{q}_3)\}\\ &\quad + \text{cyclic}\end{aligned} \tag{39}$$

is the Jacobiator for the 2-bracket {,}. It is easy to check that (38) is not satisfied. Hence the nonassociativity occurring in the topological insulator is not of the Malcev type. We remark that the closest we can get for a meaningful relation involving a Jacobiator and a 2-bracket {,} is

$$\begin{aligned}&\{\{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2),(f_3,\mathbf{q}_3)\},(f_1,\mathbf{q}_1)\}\\ &\quad = \{(f_1,\mathbf{q}_1),\{(f_2,\mathbf{q}_2),(f_1,\mathbf{q}_1)\},(f_3,\mathbf{q}_3)\}\\ &\qquad + \{(f_1,\mathbf{q}_1),(f_2,\mathbf{q}_2),\{(f_3,\mathbf{q}_3),(f_1,\mathbf{q}_1)\}\}\\ &\qquad + \big(if_1^2 f_2 f_3(\mathbf{q}_1\times\mathbf{q}_2)\cdot\mathbf{q}_3\,(\mathbf{q}_1\cdot\nabla)(\nabla\cdot\mathbf{B}),\\ &\qquad \times 2\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3\big).\end{aligned} \tag{40}$$

There is however not a simple type of nonassociativity that one can associate this with.

What about a relation involving two Jacobiators? In the literature, given an algebra $\mathscr{A}$ with a multilinear and completely antisymmetric 3-bracket $\{\cdot,\cdot,\cdot\}:\mathscr{A}\otimes\mathscr{A}\otimes\mathscr{A}\to\mathscr{A}$, the 3-bracket is said to satisfy the *fundamental identity* if the bracket of the bracket satisfies the relation

$$\begin{aligned}\{\{x_1,x_2,x_3\},x_4,x_5\} &= \{\{x_1,x_4,x_5\},x_2,x_3\} + \{x_1,\{x_2,x_4,x_5\},x_3\}\\ &\quad + \{x_1,x_2,\{x_3,x_4,x_5\}\}\end{aligned} \tag{41}$$

for arbitrary $x_1,\ldots,x_5 \in \mathscr{A}$. The fundamental identity is a natural generalization of the *Jacobi identity*

$$\{\{x_1,x_2\},x_3\} = \{\{x_1,x_3\},x_2\} + \{x_1,\{x_2,x_3\}\} \tag{42}$$

for the antisymmetric 2-bracket $\{\cdot,\cdot\}:\mathscr{A}\otimes\mathscr{A}\to\mathscr{A}$. The fundamental identity is an important consistency condition which allows for the introduction of a symmetry transformation of the algebra. Just as an antisymmetric 2-bracket which satisfies the Jacobi identity (42) can be used to define a homeomorphism of the algebra

$$\delta X := \{a,X\},\quad a,X\in\mathscr{A}, \tag{43}$$

which acts as a derivation on the 2-bracket

$$\delta\{X,Y\} = \{\delta X,Y\} + \{X,\delta Y\}, \tag{44}$$

a 3-bracket which satisfies the the fundamental identity (41) can be used to generate a homeomorphism of the algebra

$$\delta X := \{a,b,X\},\quad a,X\in\mathscr{A}. \tag{45}$$

This acts as a derivation on the 3-bracket

$$\delta\{X,Y,Z\} = \{\delta X,Y,Z\} + \{X,\delta Y,Z\} + \{X,Y,\delta Z\} \tag{46}$$

and can thus be considered as a symmetry transformation of the algebra.

The simplest example of a 3-bracket which satisfies the fundamental identity is the canonical Nambu bracket $\{f,g,h\} := \epsilon^{ijk}\partial_i f\partial_j g\partial_k h$ defined for any functions f,g,h over a 3-dimensional manifold [37]. In general a Nambu bracket is a completely antisymmetric 3-bracket which satisfies the fundamental identity (41). It is straightforward to check that the Jacobiator (24) for any three $x_i = (f_i,\mathbf{q}_i), i = 1,2,3,$ indeed satisfies the fundamental identity (41). As a result, the Jacobiator (25) also satisfies the fundamental identity

$$\begin{aligned}&[[\mathcal{O}_1,\mathcal{O}_2,\mathcal{O}_3],\mathcal{O}_4,\mathcal{O}_5]\\ &\quad = [[\mathcal{O}_1,\mathcal{O}_4,\mathcal{O}_5],\mathcal{O}_2,\mathcal{O}_3] + [\mathcal{O}_1,[\mathcal{O}_2,\mathcal{O}_4,\mathcal{O}_5],\mathcal{O}_3]\\ &\qquad + [\mathcal{O}_1,\mathcal{O}_2,[\mathcal{O}_3,\mathcal{O}_4,\mathcal{O}_5]],\end{aligned} \tag{47}$$

where $\mathcal{O}_n$ denotes the operator $\mathcal{O}(f_n,\mathbf{q}_n)$. Hence our nonassociative geometry, characterized by the Jacobiator (25), is a Nambu bracket and we call this a nonassociative Nambu geometry.

We remark that the notion of a Nambu bracket as one characterized by the fundamental identity was originally introduced by Nambu in his formulation of a generalized mechanics [37]. In the same paper Nambu also considered the quantization problem of the classical Nambu mechanics and considered the completely antisymmetrizer as a candidate for a quantization of the canonical Nambu bracket. This 3-bracket was considered in [27]. We also remark that in some applications, e.g., in the generalization of the Hamiltonian mechanics known as the Nambu mechanics [47], it is useful to introduce the notion of a Nambu-Poisson bracket, which is defined for an algebra with a binary product $\circ$ to be a completely antisymmetric 3-bracket which satisfies in addition to the fundamental identity also the derivation rule:

$$\{x_1,x_2,y_1\circ y_2\} = y_1\circ\{x_1,x_2,y_2\} + \{x_1,x_2,y_1\}\circ y_2. \quad (48)$$

This is not what we considered here.

III. NONASSOCIATIVE UNCERTAINTY RELATION

For a noncommutative geometry defined by a commutation relation

$$[X,Y] = i\theta, \quad (49)$$

it is easy to derive an associated uncertainty relation constraining the quantum fluctuation of the operators. If X,Y are Hermitian, the noncommutative uncertainty relation takes the form

$$\delta X\ \delta Y \geqslant \tfrac{1}{2}|\langle[X,Y]\rangle|. \quad (50)$$

This gives a constraint on the root-mean-square deviation of the operators

$$\delta X := \sqrt{\langle(\Delta X)^2\rangle}, \quad \Delta X := X - \langle X\rangle, \quad (51)$$

in terms of the expectation value of the commutator of X,Y. The uncertainty relation (50) can be easily generalized to the case of non-Hermitian operators. However the generalization is not unique. For example one can write down the uncertainty relation

$$\tfrac{1}{2}(\delta X\ \delta' Y + \delta' X\ \delta Y) \geqslant \tfrac{1}{2}|\langle[X,Y]\rangle|, \quad (52)$$

or the more symmetrical form

$$\bar\delta X\ \bar\delta Y \geqslant \tfrac{1}{2}|\langle[\mathrm{Re}X,\mathrm{Re}Y]\rangle|, \quad (53)$$

where here

$$\delta X := \sqrt{\langle\Delta X^\dagger\Delta X\rangle}, \quad \delta' X := \sqrt{\langle\Delta X\Delta X^\dagger\rangle}, \quad \text{and}$$
$$\bar\delta X := \tfrac{1}{2}(\delta X + \delta' X). \quad (54)$$

The proofs of these are simple. In fact, (52) is a direct application of the Schwarz inequality $|\langle\alpha|\beta\rangle|^2 \leqslant |\langle\alpha|\alpha\rangle||\langle\beta|\beta\rangle|$, for arbitrary states $|\alpha\rangle,|\beta\rangle$. Similar inequalities can be obtained for $|\langle[X^\dagger,Y]\rangle|$, $|\langle[X,Y^\dagger]\rangle|$, $|\langle[X^\dagger,Y^\dagger]\rangle|$, and the inequality (53) is obtained by adding them together.

For our case, the Schwarz inequality is still valid since associativity of the operator product was not needed in the proof of it. Therefore we can apply, for example, the uncertainty relation (53) to the commutation relation (11) and obtain the "volume" uncertainty relation

$$\bar\delta\hat\rho_{\mathbf{q}_1}\bar\delta\hat\rho_{\mathbf{q}_2}\bar\delta\hat\rho_{\mathbf{q}_3} \geqslant \sqrt{\frac{|\langle\theta_{\mathbf{q}_1\mathbf{q}_2}\rangle\langle\theta_{\mathbf{q}_1\mathbf{q}_3}\rangle\langle\theta_{\mathbf{q}_2\mathbf{q}_3}\rangle|}{8}}, \quad (55)$$

where $\theta_{\mathbf{q}_1\mathbf{q}_2} = (E_{\mathbf{q}_1\mathbf{q}_2} + E_{\mathbf{q}_1-\mathbf{q}_2} + E_{-\mathbf{q}_1\mathbf{q}_2} + E_{-\mathbf{q}_1-\mathbf{q}_2})/4$ and $E_{\mathbf{q}_1\mathbf{q}_2}$ is given by the right-hand side of (11) divided by i. Note however that this is purely a consequence of the commutation relation. In our case, we have also a nonassociative geometry with the Jacobiator relation

$$[X,Y,Z] = i\theta. \quad (56)$$

Our goal is to extract the associated uncertainty relation that is a consequence of the presence of nonassociativity.

Writing $[X,Y,Z] = [\Delta X,\Delta Y,\Delta Z]$ and denoting $A_{XY} := \Delta X\Delta Y$, $A_{YX} := \Delta Y\Delta X$, etc., we have

$$|\langle\theta\rangle| \leqslant |\langle[A_{XY},\Delta Z]\rangle| + |\langle[A_{YX},\Delta Z]\rangle| + (X,Y,Z\ \text{cyclic}). \quad (57)$$

Using (52), we have

$$\tilde\delta A_{XY}\ \delta' Z + \tilde\delta' A_{XY}\ \delta Z + (X,Y,Z\ \text{cyclic}) \geqslant \frac{|\langle\theta\rangle|}{2}, \quad (58)$$

where δZ, $\delta' Z$ are given by (54) and

$$\tilde\delta A_{XY} := \tfrac{1}{2}(\delta A_{XY} + \delta A_{YX}), \quad \tilde\delta' A_{XY} := \tfrac{1}{2}(\delta' A_{XY} + \delta' A_{YX}), \quad (59)$$

etc. The relation (58) gives a lower bound constraint on the product of the coordinate uncertainties, $\delta X,\delta' X,\ldots$, and of the "area" uncertainties, $\tilde\delta A_{XY},\tilde\delta' A_{XY},\ldots$. Since (56) is invariant under the rotation group acting on X,Y,Z, it is desirable to have a form of the uncertainty relation that is manifestly expressed in terms of SO(3)-invariant quantities. To do this, let us utilize the inequality $\sum x_i y_i \leqslant \sqrt{\sum x_i^2}\sqrt{\sum y_i^2}$ for real x_i,y_i and obtain from (58)

$$\hat\delta R\ \hat\delta A \geqslant \frac{|\langle\theta\rangle|}{4}, \quad (60)$$

where

$$(\hat\delta R)^2 := (\delta_r X)^2 + (\delta_r Y)^2 + (\delta_r Z)^2 \quad \text{with}$$
$$(\delta_r O)^2 := \frac{(\delta O)^2 + (\delta' O)^2}{2} \quad (61)$$

and

$$(\hat\delta A)^2 := \frac{(\tilde\delta A_{XY})^2 + (\tilde\delta' A_{XY})^2}{2} + \frac{(\tilde\delta A_{YZ})^2 + (\tilde\delta' A_{ZY})^2}{2} + \frac{(\tilde\delta A_{ZX})^2 + (\tilde\delta' A_{XZ})^2}{2}. \quad (62)$$

In the special case where X,Y,Z are Hermitian, $\delta_r O = \delta O$, $\tilde\delta A_{XY} = \tilde\delta' A_{XY}$,

$$(\hat\delta R)^2 = (\delta X)^2 + (\delta Y)^2 + (\delta Z)^2, \quad (63)$$

and

$$(\hat\delta A)^2 = (\tilde\delta A_{XY})^2 + (\tilde\delta A_{YZ})^2 + (\tilde\delta A_{ZX})^2. \quad (64)$$

Due to their origin, we will call (58), (60) *nonassociative uncertainty relations*.

In our case, taking $(X,Y,Z) = (\rho_{\mathbf{q}_1}, \rho_{\mathbf{q}_2}, \rho_{\mathbf{q}_3})$, let us evaluate the lower bound for the constraint (60). Assuming that we have monopoles of charge Q_n at the position $\mathbf{k}_n = \boldsymbol{\zeta}_n$ in the BZ, it is $\sum_n Q_n = 0$ according to the Nielsen-Ninomiya theorem. Evaluating the delta function, we obtain in the leading order of small momentum the following expression for the lower bound for the nonassociative uncertainty relations (58), (60):

$$|\langle\theta\rangle| = |(\mathbf{q}_1 \times \mathbf{q}_2) \cdot \mathbf{q}_3| \left| \sum_n Q_n \langle N_n^\alpha \rangle \right|, \tag{65}$$

where $N_n^\alpha := N_{\zeta_n}^\alpha$ and $N_{\mathbf{k}}^\alpha = \gamma_{\mathbf{k}}^{\alpha\dagger}\gamma_{\mathbf{k}}^\alpha$ is the number operator for the orbital creation operator. As the expression (65) depends only on simple properties of the Weyl node, we expect to extract interesting information from these uncertainty relations. This will be the subject for further work.

In this paper, we have pointed out the presence of nonassociativity in the algebra of density operators in a Weyl semimetal. This breakdown of associativity can be thought of as some kind of "anomaly," with the fundamental identity playing the role of the consistency condition. The nonassociativity is supported by the monopoles situated at the Weyl nodes, which are also exactly where the Fermi arcs end. Since Fermi arcs played a very important role in the spectral flow between the Weyl points, it will be interesting to relate the algebraic structure of the projected density operators to the properties of Fermi arcs and related spectral flow. It will also be interesting to apply the algebraic structure to derive the spectral sum rules for the density correlation functions for Weyl semimetals [48].

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