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Noncommutative geometry for three-dimensional topological insulators

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We generalize the noncommutative relations obeyed by the guiding centers in the two-dimensional quantum Hall effect to those obeyed by the projected position operators in three-dimensional (3D) topological band insulators. The noncommutativity in 3D space is tied to the integral over the 3D Brillouin zone of a Chern-Simons invariant in momentum-space. We provide an example of a model on the cubic lattice for which the chiral symmetry guarantees a macroscopic number of zero-energy modes that form a perfectly flat band. This lattice model realizes a chiral 3D noncommutative geometry. Finally, we find conditions on the density-density structure factors that lead to a gapped 3D fractional chiral topological insulator within Feynman's single-mode approximation.

I. INTRODUCTION

The integer quantum Hall effect (IQHE)[1] is the first known example of a fermionic phase of matter characterized by a topological index that is directly connected to a physical observable. The index in this case is the sum of the (first) Chern numbers obtained for each of the fully filled Landau bands, and the associated physical observable is the Hall conductance.[2–4] The fractional quantum Hall effect (FQHE) [5] results from the effects of electron-electron interactions when the Landau levels are partially filled with electrons, for certain rational filling fractions.[6] More examples of topological states of matter that are comprised of noninteracting fermions have been discovered recently,[7–16] and have been classified according to discrete symmetries they respect or not, and the dimensionality of space in which the particles propagate.[17–19] Such classification is sometimes referred to as the "periodic table" of topological insulators.[18] Among these states are $\mathbb{Z}_2$ topological ones associated with the presence of time-reversal symmetry (TRS) in two-dimensional (2D) as well as three-dimensional (3D) systems. It is natural to then question what the "fractional" version of these phases should be, and how they could be described. In particular, it is interesting to ask what are the possible fractional topological phases of interacting fermionic systems in three spatial dimensions.

One approach to capture universal physics arising from topological interacting electron systems in $(2+1)$[20–27] and $(3+1)$[28–30] dimensions of space and time is via the parton construction. A fractional phase of electrons is obtained by constructing integer filled bands of "partons", which are then "glued" together by very strong gauge-mediated interactions so as to assemble together the physical electron. This approach is a generalization of theories that capture the universal physics of the FQHE, and yields, for instance, wavefunctions describing states that support fractional magneto-electric effects [28–30] in the case of the $\mathbb{Z}_2$ topological insulators. The parton construction is one way to obtain an effective topological quantum field theory (TQFT) to describe fractional topological insulators.

However, TQFTs do not capture the dynamics of the systems beyond their topological properties. As emphasized by Haldane,[31] TQFTs are incomplete theories of the FQHE, for while they characterize the quantum numbers of the elementary excitations (topological defects), such as their charges and statistics, they do not contain any information about their energies. The information about the fundamental length scale in the FQHE, the magnetic length, is lost in its TQFT treatment. Recently Haldane has proposed in Refs. 31 and 32 a geometric description of the FQHE based on the algebra obeyed by the density operators projected to the lowest Landau level that was originally introduced by Girvin, MacDonald and Platzman (GMP) in Ref. 33.

When projected to the lowest Landau level, the density operators do not commute. However, the algebra closes in that the commutation of two density operators is proportional to a third one. Using this algebra, GMP were able to employ an approach that parallels that of Feynman and Bijl in their study of excitations in ^{4}He.[34] Their approach allows to place a variational estimate on the excitation gap, if the static structure factor is known. The algebraic approach to the FQHE pioneered by GMP has also been useful to understand the hydrodynamic description of the edge states in the IQHE and FQHE.[35–37] More recently, Parameswaran, Roy, and Sondhi in Ref. 38 have initiated a study of the algebra obeyed by the density operators in two-dimensional Chern band insulators (see also Refs. 39 and 40). Our work in 3D is motivated by this successful approach in 2D.

The main objective of this work is to identify the noncommutative geometry that can emerge from 3D topological insulators, its relation to topological invariants, and its relevance to possible interaction-driven topological fractional phases in fermionic 3D systems. Armed with this noncommutative geometry, one can forge ahead in trying to construct a dynamical theory of 3D fractional topological insulators that could, perhaps, parallel the solid understanding of the FQHE in 2D. In particu-

lar, the approach might suggest which types of interactions can give rise to incompressible gapped phases and support the counterparts to the magneto-roton collective excitation in the FQHE.[33]

There are important symmetry considerations that need to be carefully taken into account when searching for interacting topological insulators in 3D. The FQHE descends from the IQHE when Landau or Chern bands are partially filled. In turn, the 2D IQHE is a stable class of states characterized by a $\mathbb{Z}$ index (symmetry class A in the terminology of Ref. 17), which has no symmetry left out to be broken. If the logic is that we are also to start from a noninteracting topological insulator in 3D when constructing the interacting fractional counterpart, we need to look at systems which are topologically nontrivial in 3D space. One possibility is to start with $\mathbb{Z}_2$ topological insulators. This has been the choice in most works so far. Here, instead, we shall start from systems that have chiral symmetry, but lack TRS (symmetry class AIII in the terminology of Ref. 17). The rational for this choice is twofold. First, from experience working on strongly interacting 2D $\mathbb{Z}_2$ topological insulators, we have observed that TRS is easily broken in favor of magnetized states due to the Stoner instability, which is enhanced in bands with nonzero topological invariant.[41–43] Second, because 3D chiral systems are characterized by a $\mathbb{Z}$-valued topological invariant, they might share similarities with the FQHE. Indeed, we shall show that the noncommutative geometry for this 3D model does depend on this $\mathbb{Z}$-valued topological invariant.

The approach of GMP is ideally suited to the situation where density operators are projected into a dispersionless band (for example the lowest Landau level in the case of the FQHE). Here, we shall give a concrete lattice model with chiral symmetry that contains an exactly flat topological band, on which we construct the projected density operators. The resulting operator product expansions will depend on the nonzero integral over the 3D Brillouin zone of a Chern-Simons action in momentum-space. For this lattice model, the average Berry curvature over the entire Brillouin zone is zero. Hence, the type of 3D fractional topological insulator that we discuss is qualitatively different from the FQHE, where the average Berry curvature over the Brillouin zone is nonzero. The nature of the fractional states we discuss are intrinsically 3D, and not layered 2D (i.e., weak topological insulators).

The main results of this paper are the following.

In Sec. II, we relate algebraic and topological properties of noninteracting fermions assuming a translation-invariant insulating ground state. Although we are mostly interested in either 2D or 3D space, our method applies to any dimension d of space. We show in Sec. II A that the position operators for noninteracting fermions, if projected onto the occupied bands that make up the insulating Fermi sea, obey a noncommutative geometry that is tied to the single-particle band topology. More precisely, for any 3D translation-invariant and non-interacting fermionic Hamiltonian with an insulating Fermi sea as ground state, Eq. (2.54) relates the ground state expectation value of the 3-bracket for the projected position operators to Chern-Simons invariants in 1D and 3D momentum space. If we impose chiral symmetry, Eq. (2.55) dictates that it is only the Chern-Simons invariant in 3D momentum space that controls this ground state expectation value. Imposing chiral symmetry is thus a mean by which intrinsic 3D physics marries noncommutative geometry with band topology. We show in Sec. II B with the help of Eq. (2.65) how to relate the noncommutative geometry obeyed by the position operator to that obeyed by the translation operator in momentum space by means of an operator product expansion, whenever chiral symmetry holds. The results of Sec. II A are applied to the case of a 3D Dirac Hamiltonian in Sec. II C. This 3D Dirac Hamiltonian can be thought of as playing the role of the Landau Hamiltonian in 2D space. So far, the position operators under consideration are always unbounded operators. Hence, Eqs. (2.55) and (2.65) are not applicable to tight-binding (lattice) models. Section II D treats the operator product expansion for the Fourier modes in momentum space of the fermion density operator when projected onto a single band. As opposed to the unbounded position operators from Sec. II A, there is no direct relation between the 3-bracket of the projected density operators and band topology. Instead, the interplay between algebra and band topology is captured by Eq. (2.88) for any 3D lattice model with chiral symmetry.

A minimal microscopic 3D noninteracting lattice Hamiltonian that realizes the conditions necessary to marry the noncommutative geometry to the band topology of Sec. II is presented in Sec. III. A noninteracting fermionic 3-band (of which one is flat) Hamiltonian is defined in Sec. III A. The band topology is characterized by three distinct topological numbers defined in Sec. III B by Eqs. (3.7), (3.10), and (3.12), respectively. They are related by Eq. (3.14). Bulk band topology implies the existence of boundary states that disperse across the bulk band gap in open geometries and to which we devote Sec. III C.

The role of density-density interactions for screened Coulomb interactions is discussed in Sec. IV for tight-binding models on d-dimensional lattices within the single-mode approximation (SMA) under the assumption that there exists at least one flat band in the noninteracting limit. We follow GMP and construct a family of variational states labeled by momentum through the application of the Fourier modes in momentum space of the projected (on the flat band) fermion density operator on the exact interacting many-body ground state. The corresponding variational energy dispersion then delivers, within this approximation, the condition(s) for or against the existence of a gap or the existence of collective modes, as was achieved assuming a Laughlin state for the exact ground state in the FQHE by GMP. If we denote the variational excitation energy by the fraction $\Delta(\boldsymbol{k}) = f(\boldsymbol{k})/s(\boldsymbol{k})$, where both the denominator and numerator are expectation values with a variational

state such that the denominator turns out to be the static structure factor of the exact interacting many-body ground state, we show with the help of Eq. (4.10) the conditions under which $f(\boldsymbol{k}) \sim \boldsymbol{k}^2$ for 2D and 3D lattice models. A variational gap then requires that the static structure factor $s(\boldsymbol{k})$ of the exact many-body ground state scales like $s(\boldsymbol{k}) \sim \boldsymbol{k}^2$ within the SMA. The condition $s(\boldsymbol{k}) \sim \boldsymbol{k}^2$ for a SMA gap can be tested numerically given any Ansatz for the many-body ground state.

II. NONCOMMUTATIVE GEOMETRY

We begin by recalling some elementary facts about the quantum motion of a spinless electron confined to move in the plane spanned by the orthonormal unit vectors $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ perpendicular to an applied uniform magnetic field $\boldsymbol{B} = B\,\boldsymbol{e}_3$, whereby $\boldsymbol{e}_3 = \boldsymbol{e}_1 \wedge \boldsymbol{e}_2$.

Its quantum dynamics is governed by the single-particle (Landau) Hamiltonian

$$\widehat{\mathcal{H}} := \frac{1}{2m_{\rm e}} \left[\widehat{\boldsymbol{P}} + \frac{e}{c} \boldsymbol{A}(\widehat{\boldsymbol{R}}) \right]^2, \qquad \boldsymbol{B} = \boldsymbol{\nabla} \wedge \boldsymbol{A}(\boldsymbol{r}), \quad (2.1)$$

where the momentum $\widehat{\boldsymbol{P}}^{\mathsf{T}} \equiv (\widehat{P}_1, \widehat{P}_2)$ and position $\widehat{\boldsymbol{R}}^{\mathsf{T}} \equiv (\widehat{R}_1, \widehat{R}_2)$ operators obey the canonical commutation relation

$$\left[\widehat{R}_\mu, \widehat{P}_\nu \right] = {\rm i}\hbar\, \delta_{\mu,\nu} \quad (2.2)$$

with $\mu, \nu = 1, 2$.

Hence, neither do the components of the covariant derivative in position space

$$\widehat{\boldsymbol{\Pi}} := \frac{{\rm i}m_{\rm e}}{\hbar} \left[\widehat{\mathcal{H}}, \widehat{\boldsymbol{R}} \right] = \widehat{\boldsymbol{P}} + \frac{e}{c} \boldsymbol{A}(\widehat{\boldsymbol{R}}) \quad (2.3a)$$

nor do the components of the conserved guiding center

$$\widehat{\boldsymbol{X}} := \widehat{\boldsymbol{R}} - \frac{\ell_B^2}{\hbar} \boldsymbol{e}_3 \wedge \widehat{\boldsymbol{\Pi}} \quad (2.3b)$$

commute, for

$$\left[\widehat{\Pi}_1, \widehat{\Pi}_2 \right] = -{\rm i} \frac{\hbar^2}{\ell_B^2} \quad (2.4a)$$

and

$$\left[\widehat{X}_1, \widehat{X}_2 \right] = +{\rm i}\, \ell_B^2 \quad (2.4b)$$

with $\ell_B = \sqrt{\hbar c/(eB)}$ the magnetic length.

An orthonormal basis of energy eigenstates of the Landau Hamiltonian (2.1) is made of the kets

$$|n, m\rangle := \frac{1}{\sqrt{n!m!}} (\widehat{a}^\dagger)^n (\widehat{b}^\dagger)^m |0\rangle, \quad (2.5a)$$

with

$$\widehat{a}^\dagger := \frac{\ell_B}{\sqrt{2}\hbar} \left(\widehat{\Pi}_1 + {\rm i}\widehat{\Pi}_2 \right), \quad \widehat{b}^\dagger := \frac{1}{\sqrt{2}\,\ell_B} \left(\widehat{X}_1 + {\rm i}\widehat{X}_2 \right), \quad (2.5b)$$

and where $n = 0, 1, 2, \cdots$ labels the Landau levels with energy $\varepsilon_n = \hbar\omega_c\,(n+1/2)$ and $m = 0, 1, 2, \cdots, [(\Phi/\Phi_0) - 1]$ labels the orbital angular momentum. Here, $\Phi = AB$ is the magnetic flux threading the area A of the system, $\Phi_0 = hc/e$ is the flux quantum, and $\omega_c = eB/m_{\rm e}c$ is the cyclotron frequency.

Defining the projector on the n-th Landau level

$$\widehat{\mathcal{P}}_n := \sum_m |n, m\rangle\langle n, m|, \quad (2.6)$$

one finds that the guiding center defined in Eq. (2.3b) is the position operator projected on any single Landau level

$$\begin{aligned} \widehat{\boldsymbol{X}} &= \frac{\ell_B}{\sqrt{2}} \begin{pmatrix} \widehat{b} + \widehat{b}^\dagger \\ {\rm i}\widehat{b} - {\rm i}\widehat{b}^\dagger \end{pmatrix} \\ &= \frac{\ell_B}{\sqrt{2}} \widehat{\mathcal{P}}_n \left[\begin{pmatrix} \widehat{b} + \widehat{b}^\dagger \\ {\rm i}\widehat{b} - {\rm i}\widehat{b}^\dagger \end{pmatrix} - \begin{pmatrix} {\rm i}\widehat{a}^\dagger - {\rm i}\widehat{a} \\ \widehat{a}^\dagger + \widehat{a} \end{pmatrix} \right] \widehat{\mathcal{P}}_n \\ &= \widehat{\mathcal{P}}_n\, \widehat{\boldsymbol{R}}\, \widehat{\mathcal{P}}_n, \end{aligned} \quad (2.7)$$

since $\widehat{\mathcal{P}}_n\, \widehat{a}\, \widehat{\mathcal{P}}_n = 0$ and $\widehat{\mathcal{P}}_n\, \widehat{a}^\dagger\, \widehat{\mathcal{P}}_n = 0$, while $\widehat{\mathcal{P}}_n\, \widehat{b}\, \widehat{\mathcal{P}}_n = \widehat{b}$ and $\widehat{\mathcal{P}}_n\, \widehat{b}^\dagger\, \widehat{\mathcal{P}}_n = \widehat{b}^\dagger$. Thus, the position operators projected to any given Landau level satisfy the noncommutative geometry (2.4b).

This noncommutative geometry is at the heart of both the IQHE and the FQHE. For example, it is intimately related to the quantized Hall conductivity $\sigma^{\rm H}$. The Kubo formula for the contribution of the n-th Landau level ($n = 0, 1, 2, \cdots$) to the Hall conductivity is

$$\sigma_n^{\rm H} := \frac{e^2\hbar}{{\rm i}m_{\rm e}^2} \frac{1}{A} \sum_{n' \neq n} \sum_m \frac{\langle n, m|\widehat{\Pi}_1 \widehat{\mathcal{P}}_{n'} \widehat{\Pi}_2 |n, m\rangle - (1 \leftrightarrow 2)}{(\varepsilon_n - \varepsilon_{n'})^2}, \quad (2.8)$$

where A is the area of the Hall droplet. This can be rewritten using Eq. (2.3a) as

$$\begin{aligned} \sigma_n^{\rm H} &= \frac{{\rm i}e^2}{A\hbar} \sum_{n' \neq n} \sum_m \left[\langle n, m|\widehat{R}_1 \widehat{\mathcal{P}}_{n'} \widehat{R}_2 |n, m\rangle - (1 \leftrightarrow 2) \right] \\ &= -\frac{{\rm i}e^2}{A\hbar} \sum_m \left[\langle n, m|\widehat{R}_1 \widehat{\mathcal{P}}_n \widehat{R}_2 |n, m\rangle - (1 \leftrightarrow 2) \right] \\ &= -\frac{{\rm i}e^2}{A\hbar} \sum_m \left\langle n, m \left| \left[\widehat{X}_1, \widehat{X}_2 \right] \right| n, m \right\rangle \\ &= \frac{e^2}{h}, \end{aligned} \quad (2.9)$$

where we used that $A = 2\pi \sum_m \ell_B^2$. The role of the noncommutative position-operator algebra is apparent in the penultimate line.

To quadratic order in ℓ_B, the algebra of the projected position operators (2.3b) is maintained if a coordinate transformation $r_\mu \to f_\mu(\boldsymbol{r})$, $\mu = 1, 2$, that varies on length scales larger than ℓ_B, is area preserving. Indeed, we can then expand

$$\left[f_1(\widehat{\boldsymbol{X}}), f_2(\widehat{\boldsymbol{X}})\right] = +\mathrm{i}\,\ell_B^2\,\{f_1, f_2\}_{\mathrm{P}}\,(\widehat{\boldsymbol{X}}) + \mathcal{O}\left(\ell_B^4\right), \tag{2.10a}$$

where the classical Poisson bracket is defined as

$$\{f_1, f_2\}_{\mathrm{P}}\,(\boldsymbol{r}) := \epsilon^{\mu\nu}\left(\frac{\partial f_1}{\partial r_\mu}\frac{\partial f_2}{\partial r_\nu}\right)(\boldsymbol{r}). \tag{2.10b}$$

The condition for this coordinate transformation to locally preserve area is that its Jacobian equals unity, or equivalently that $\{f_1, f_2\}_{\mathrm{P}}\,(\boldsymbol{r}) = 1$. In this case, it follows that $\left[f_1(\widehat{\boldsymbol{X}}), f_2(\widehat{\boldsymbol{X}})\right] = +\mathrm{i}\,\ell_B^2 + \mathcal{O}(\ell_B^4)$.

From the projected coordinate algebra, one can obtain a (projected) density algebra, by defining the projected density

$$\widehat{\rho}(\boldsymbol{r}) := \widehat{\mathcal{P}}_n\,\widehat{\varrho}(\boldsymbol{r})\,\widehat{\mathcal{P}}_n, \tag{2.11a}$$

where the unprojected density operator is

$$\widehat{\varrho}(\boldsymbol{r}) := \delta\left(\boldsymbol{r} - \widehat{\boldsymbol{R}}\right). \tag{2.11b}$$

One can also construct the guiding center operators (2.3b) from the projected density operators through

$$\widehat{X}_\mu = \int \mathrm{d}^2\boldsymbol{r}\, r_\mu\,\widehat{\mathcal{P}}_n\,\widehat{\varrho}(\boldsymbol{r})\,\widehat{\mathcal{P}}_n, \qquad \mu = 1, 2. \tag{2.12}$$

In momentum space, the projected normal ordered density operators

$$\begin{aligned}\widehat{\rho}(\boldsymbol{q}) &:= e^{\ell_B^2\boldsymbol{q}^2/4}\,\widehat{\mathcal{P}}_0 :e^{\mathrm{i}\boldsymbol{q}\cdot\widehat{\boldsymbol{R}}}: \widehat{\mathcal{P}}_0 \\ &= e^{\mathrm{i}\boldsymbol{q}\cdot\widehat{\boldsymbol{X}}}\end{aligned} \tag{2.13}$$

in the lowest Landau level $n = 0$ satisfy the commutation relations [33]

$$[\widehat{\rho}(\boldsymbol{q}_1), \widehat{\rho}(\boldsymbol{q}_2)] = -2\,\mathrm{i}\,\sin\left(\frac{\ell_B^2}{2}\,(\boldsymbol{q}_1 \wedge \boldsymbol{q}_2)\cdot\boldsymbol{e}_3\right)\widehat{\rho}(\boldsymbol{q}_1 + \boldsymbol{q}_2) \tag{2.14a}$$

or, in the limit of small momenta $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$,

$$[\widehat{\rho}(\boldsymbol{q}_1), \widehat{\rho}(\boldsymbol{q}_2)] \approx -\mathrm{i}\,\ell_B^2\;(\boldsymbol{q}_1 \wedge \boldsymbol{q}_2)\cdot\boldsymbol{e}_3\,\widehat{\rho}(\boldsymbol{q}_1 + \boldsymbol{q}_2), \tag{2.14b}$$

or, equivalently, to lowest order in the $\boldsymbol{q}$'s,

$$\left[\partial_{q_1^\mu}\widehat{\rho}\,(\boldsymbol{q}_1), \partial_{q_2^\nu}\widehat{\rho}\,(\boldsymbol{q}_2)\right] \approx -\mathrm{i}\,\ell_B^2\,\epsilon_{\mu\nu}\,\widehat{\rho}(\boldsymbol{q}_1 + \boldsymbol{q}_2). \tag{2.14c}$$

This algebra, the GMP algebra,[44–48] plays two crucial roles. First, within the SMA approximation,[33] it dictates under what conditions interactions open a spectral gap between the many-body interacting ground state and its excitations upon lowering the chemical potential within the first Landau level. Second, it also dictates the universal properties of the low-energy and long-distance dynamics at the edge in an open geometry.[35–37]

The goal of the work presented in the remainder of this section is to generalize the noncommutative geometry encoded by Eqs (2.4b) and (2.14c) to noninteracting many-body fermionic Hamiltonians in 3D space. Before carrying out this program, let us motivate what it is to come by first presenting what would constitute a natural extension of the algebra in the QHE to 3D problems.

First, instead of the commutator, consider the case where the 3-bracket of the 3D projected position operators equals a $\mathbb{C}$-number

$$\left[\widehat{X}_1, \widehat{X}_2, \widehat{X}_3\right] = \mathrm{i}\,\ell^3, \tag{2.15a}$$

where, following Nambu,[49] we have defined the 3-bracket

$$\begin{aligned}[\widehat{A}_1, \widehat{A}_2, \widehat{A}_3] &:= \epsilon^{ijk}\widehat{A}_i\widehat{A}_j\widehat{A}_k \\ &= [\widehat{A}_1, \widehat{A}_2]\,\widehat{A}_3 + [\widehat{A}_2, \widehat{A}_3]\,\widehat{A}_1 + [\widehat{A}_3, \widehat{A}_1]\,\widehat{A}_2.\end{aligned} \tag{2.15b}$$

The characteristic length scale ℓ of the 3D noninteracting many-body Hamiltonian, not to be confused with the magnetic length ℓ_B of the 2D Landau Hamiltonian, is the signature of a spectral gap separating the ground state from the excited states. Similarly to the 2D case, for which area preserving coordinate transformations leave the commutation relations unchanged, we would like volume preserving transformations not to change the 3-bracket. Under generic transformations $r_\mu \to f_\mu(\boldsymbol{r})$, $\mu = 1, 2, 3$, that vary on length scales larger than ℓ,

$$\left[f_1(\widehat{\boldsymbol{X}}), f_2(\widehat{\boldsymbol{X}}), f_2(\widehat{\boldsymbol{X}})\right] = \mathrm{i}\,\ell^3\,\{f_1, f_2, f_3\}_{\mathrm{N}}\,(\widehat{\boldsymbol{X}}) + \mathcal{O}(\ell^5), \tag{2.16a}$$

where the classical Nambu bracket is defined as [49]

$$\{f_1, f_2, f_3\}_{\mathrm{N}}\,(\boldsymbol{r}) := \epsilon^{\mu\nu\lambda}\left(\frac{\partial f_1}{\partial r^\mu}\frac{\partial f_2}{\partial r^\nu}\frac{\partial f_3}{\partial r^\lambda}\right)(\boldsymbol{r}). \tag{2.16b}$$

The condition for this coordinate transformation to locally preserve volume is that its Jacobian equals unity, or equivalently that $\{f_1, f_2, f_3\}_{\mathrm{N}}\,(\boldsymbol{r}) = 1$. In this case, it follows that $\left[f_1(\widehat{\boldsymbol{X}}), f_2(\widehat{\boldsymbol{X}}), f_3(\widehat{\boldsymbol{X}})\right] = \mathrm{i}\,\ell^3 + \mathcal{O}(\ell^5)$.

Second, we claim (and show in this paper) that the 3D counterpart to the operator product expansion (2.14) of the projected densities is, to lowest order in the $\boldsymbol{q}$'s,

$$\left[\partial_{q_1^\mu}\widehat{\rho}\,(\boldsymbol{q}_1), \partial_{q_2^\nu}\widehat{\rho}\,(\boldsymbol{q}_2), \partial_{q_3^\lambda}\widehat{\rho}\,(\boldsymbol{q}_3)\right] \approx \epsilon_{\mu\nu\lambda}\,\ell^3\,\widehat{\rho}(\boldsymbol{q}_1 + \boldsymbol{q}_2 + \boldsymbol{q}_3). \tag{2.17}$$

The algebra defined by Eqs. (2.15) and (2.17), if it can be realized by a 3D fermionic noninteracting many-body Hamiltonian, might then deliver two results. First, within the SMA approximation, it might dictate under what conditions interactions open a spectral gap between the many-body interacting ground state and its excitations upon lowering the chemical potential below the

single-particle gap. Second, it might also dictate the universal properties of the low-energy and long-distance dynamics at the boundary in an open geometry.

The key idea to realize the algebra defined by Eqs. (2.15) and (2.17) is to replace the effect of the magnetic field in the Landau Hamiltonian by that of the projection of suitable operators on a suitable subspace of the fermionic Fock space. The construction of this suitable subspace presumes the existence of fermionic Bloch bands as occurs in condensed matter physics and assumes that a subset of these bands are fully occupied, while the complementary set are empty and separated from the filled subset by an energy gap.

Now, carrying out this program for some Bloch bands will not yield immaculately the 3-brackets (2.15) and (2.17). It will yield these relations approximately in the long-wavelength limit. The situation here is similar to the case of the quantized Hall effect in flat Chern bands of 2D models.[50–53] As discussed by Parameswaran, Roy, and Sondhi in Ref. 38 (see also Refs. 39 and 40), the algebra (2.14b) follows if the fluctuations in the Berry curvature over the Brillouin zone are neglected, or equivalently if the local curvature is approximated by its average over the entire Brillouin zone. Without this approximation, however, the noncommutative relations obeyed by the projected position operator will not be as simple as in Eq. (2.4b) and may instead be represented as

$$\left[\widehat{X}_1, \widehat{X}_2\right] = \mathrm{i}\ell^2 + \cdots , \tag{2.18}$$

where $\cdots$ stands for operators that appear as a result of the inhomogeneities in the Berry curvature. The central question is how to distinguish universal from nonuniversal contributions to the right-hand side of Eq. (2.18). To answer this question, we propose to consider the ground state expectation value $\left\langle \left[\widehat{X}_1, \widehat{X}_2\right] \right\rangle$, that encodes the quantized Hall conductivity, as seen in Eq. (2.9). We show in Sec. II A that

$$\frac{1}{N_{\mathrm{p}}} \left\langle \left[\widehat{X}_1, \widehat{X}_2\right] \right\rangle = \frac{2\pi\,\mathrm{i}}{\bar{\rho}} \mathrm{Ch}^{(1)}. \tag{2.19}$$

Here, $\mathrm{Ch}^{(1)}$ is the first Chern number of the topological band that sustains the IQHE in the lattice, and will be defined in Eq. (2.53), while N_{p} is the total particle number and $\bar{\rho}$ is the average particle density. This suggests that the universal physical properties are captured by the $\mathbb{C}$-number contribution to the right-hand side of Eq. (2.18).

As with the commutator (2.18), the 3-bracket (2.15) will also acquire extra terms in 3D space

$$\left[\widehat{X}_1, \widehat{X}_2, \widehat{X}_3\right] = \mathrm{i}\,\ell^3 + \cdots . \tag{2.20}$$

We are thus lead to consider its normal ordered expectation value instead, which, as we show in Sec. II A, is given by

$$\frac{1}{N_{\mathrm{p}}} \left\langle : \left[\widehat{X}_1, \widehat{X}_2, \widehat{X}_3\right] : \right\rangle = \frac{12\pi^2\,\mathrm{i}}{\bar{\rho}}\, \mathrm{CS}^{(3)}. \tag{2.21}$$

Here, the symbol $\mathrm{CS}^{(3)}$ stands for the 3D Chern-Simons invariant defined in Eq. (2.51b). If the discrete chiral symmetry or time-reversal symmetry holds, $\mathrm{CS}^{(3)}$ is a quantized topological invariant that takes half-integer values. It is related to the dimensionless coupling

$$\theta = 2\pi \left(\mathrm{CS}^{(3)} \bmod 1\right) \tag{2.22a}$$

that enters the effective action

$$\mathcal{L}_\theta^{\mathrm{eff}} := \frac{\theta\, e^2}{4\pi^2}\, \boldsymbol{E} \cdot \boldsymbol{B} \tag{2.22b}$$

obtained from integrating out noninteracting fermions of a 3D topological insulator in the background of external electric $\boldsymbol{E}$ and magnetic $\boldsymbol{B}$ fields within linear response theory. This electro-magnetic coupling was derived by Xi, Hughes, and Zhang in Ref. 14 by dimensional reduction from a topological insulator in 4D displaying an integer quantum Hall effect to a 3D $\mathbb{Z}_2$ topological insulator (see also Ref. 54 for a generalization that accounts for moderate interactions). For a 3D $\mathbb{Z}_2$ topological insulator, time-reversal symmetry holds. In turn, time-reversal symmetry restricts θ to the two values $\theta = 0$ and $\theta = \pi$ that distinguish "ordinary" from topological 3D insulators, respectively.[14] Several derivations of the magneto-electric response, of which the θ term (2.22b) is an example, have been proposed without time-reversal symmetry.[55–59]

Equation (2.21) relates a nonvanishing $\mathrm{CS}^{(3)}$ to the noncommutative algebra obeyed by the components of the projected position operator through the noninteracting groundstate expectation value of their 3-bracket. Because the position operator and its projection are unbounded operators and because Wannier states may not be exponentially localized if the Bloch states have a topological character,[60,61] a regularization procedure is needed to compute Eq. (2.21). We shall choose a regularization that preserves gauge invariance under pure gauge transformation of the Bloch states, but that breaks a discrete translation symmetry. In doing so, we shall make a connection with Ref. 57, where a representation of the θ term is given in terms of expectation values of the position operators in the Wannier basis.

We start by deriving the conditions under which Eq. (2.21) holds in Sec. II A for any Hamiltonian that is endowed with translation invariance, a spectral gap, and describes the motion of noninteracting fermions in flat Euclidean space $\mathbb{R}^3$. We draw a connection between the 3-bracket and the (classical) Nambu bracket in Sec. II B. We then specialize in Sec. II C to the case of massive noninteracting Dirac Hamiltonians for which some analytical results can be obtained in the long-wavelength limit. Finally, Sec. II D is devoted to the operator product expansion of single-particle density operators in 3D lattice models and the conditions under which Eq. (2.17) holds.

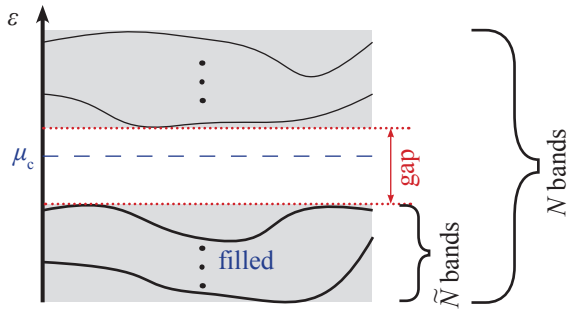

FIG. 1: (Color online) Assumed spectral gap in the single-particle energy spectrum. Here, $\mu_{\rm c}$ denotes the chemical potential and the insulating noninteracting many-body ground state $|\Phi\rangle$ is obtained by filling all the states in the $\widetilde{N}$ bands below the spectral gap.

A. Noncommutative geometry for the projected position operators

We shall consider noninteracting fermions whose dynamics are governed by the translation invariant Bloch Hamiltonian

$$\widehat{H} = \int\limits_{\Lambda^\star_{\rm BZ}} \mathrm{d}^d\boldsymbol{k} \sum_{a=1}^{N} \widehat{\chi}^\dagger_a(\boldsymbol{k})\, \varepsilon_a(\boldsymbol{k})\, \widehat{\chi}_a(\boldsymbol{k}). \tag{2.23a}$$

We are reserving the latin index $a = 1, \cdots, N$ for the band label. The momentum $\boldsymbol{k} = (k^\mu)$ belongs to the Brillouin zone

$$\Lambda^\star_{\rm BZ} := \left\{ (k^\mu) \in \mathbb{R}^d \,\middle|\, -\frac{\pi}{\mathfrak{a}} \le k^\mu < \frac{\pi}{\mathfrak{a}}, \quad \mu = 1, \cdots, d \right\} \tag{2.23b}$$

with $\pi/\mathfrak{a}$ playing the role of the upper momentum cutoff. Each band $a = 1, \cdots, N$ is characterized by the single-particle energy dispersion $\varepsilon_a(\boldsymbol{k})$, a real-valued function over the Brillouin zone. The creation and annihilation operators obey the fermionic algebra

$$\begin{aligned} \Big\{ \chi_a(\boldsymbol{k}), \chi_{a'}(\boldsymbol{k}') \Big\} &= \Big\{ \chi^\dagger_a(\boldsymbol{k}), \chi^\dagger_{a'}(\boldsymbol{k}') \Big\} = 0, \\ \Big\{ \chi_a(\boldsymbol{k}), \chi^\dagger_{a'}(\boldsymbol{k}') \Big\} &= \delta_{a,a'}\, \delta(\boldsymbol{k} - \boldsymbol{k}'), \end{aligned} \tag{2.23c}$$

for all pairs of bands and for all pairs of momenta in the Brillouin zone. Finally, for any band $a = 1, \cdots, N$, for any momentum $\boldsymbol{k}$ from the Brillouin zone, and for any Cartesian unit vector $\boldsymbol{e}^\mu$ from $\mathbb{R}^d$, we impose twisted boundary conditions across the Brillouin zone through

$$\chi_a\big(\boldsymbol{k} + (2\pi/\mathfrak{a})\, \boldsymbol{e}^\mu\big) = e^{+\mathrm{i}(2\pi\,\theta^\mu)}\, \chi_a(\boldsymbol{k}). \tag{2.23d}$$

These twisted boundary conditions are parametrized by the real numbers $0 \le \theta^\mu < 1$ with $\mu = 1, \cdots, d$.

We shall also assume that (i) there are $\widetilde{N}$ lower bands out of the N bands that are separated by an energy gap from the $N - \widetilde{N}$ remaining upper bands and (ii) the chemical potential lies in this spectral gap (see Fig. 1). We denote with

$$\widehat{P}_{\widetilde{N}} \equiv \int\limits_{\Lambda^\star_{\rm BZ}} \mathrm{d}^d\boldsymbol{k} \sum_{\tilde{a}=1}^{\widetilde{N}} \widehat{\chi}^\dagger_{\tilde{a}}(\boldsymbol{k})\, \widehat{\chi}_{\tilde{a}}(\boldsymbol{k}) \tag{2.24}$$

the projection operator on the single-particle states spanned by these gapped lower bands. We are reserving the latin index with a tilde sign $\tilde{a} = 1, \cdots, \widetilde{N}$ for the lower band labels.

In analogy to the guiding center coordinates (2.12) from the IQHE, we would like to define projected position operators. However, projected position operators are associated to gauge fields as we now explain.[62]

On the one hand, we may define the Wannier creation operator through the Fourier transform

$$\widehat{W}^\dagger_{a;\boldsymbol{R}} := \int\limits_{\Lambda^\star_{\rm BZ}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^{d/2}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\, \widehat{\chi}^\dagger_a(\boldsymbol{k}), \tag{2.25a}$$

or, equivalently, the inverse Fourier transform

$$\widehat{\chi}^\dagger_a(\boldsymbol{k}) =: \frac{1}{(2\pi/\mathfrak{a})^{d/2}} \sum_{\boldsymbol{R}\in\Lambda_R} e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\, \widehat{W}^\dagger_{a;\boldsymbol{R}}, \tag{2.25b}$$

for any band index $a = 1, \cdots, N$ and for any lattice point $\boldsymbol{R} = (R^\mu) \in \Lambda_R$ whereby

$$\Lambda_R := \left\{ (R^\mu) \in \mathbb{R}^d \,\middle|\, \frac{R^\mu}{\mathfrak{a}} = \theta^\mu \bmod 1,\ \mu = 1, \cdots, d \right\}. \tag{2.25c}$$

The length scale $\mathfrak{a}$ can thus be interpreted as a lattice spacing. Consequently, creation and annihilation Wannier operators obey the fermionic algebra

$$\begin{aligned} \Big\{ \widehat{W}_{a;\boldsymbol{R}}, \widehat{W}_{a';\boldsymbol{R}'} \Big\} &= \Big\{ \widehat{W}^\dagger_{a;\boldsymbol{R}}, \widehat{W}^\dagger_{a';\boldsymbol{R}'} \Big\} = 0, \\ \Big\{ \widehat{W}_{a;\boldsymbol{R}}, \widehat{W}^\dagger_{a';\boldsymbol{R}'} \Big\} &= \delta_{a,a'}\, \delta_{\boldsymbol{R},\boldsymbol{R}'}, \end{aligned} \tag{2.26}$$

for all pairs of bands and for all pairs of lattice sites. Moreover, the projection operator (2.24) remains diagonal in the Wannier representation (2.25),

$$\widehat{P}_{\widetilde{N}} = \sum_{\boldsymbol{R}\in\Lambda_R} \sum_{\tilde{a}=1}^{\widetilde{N}} \widehat{W}^\dagger_{\tilde{a};\boldsymbol{R}}\, \widehat{W}_{\tilde{a};\boldsymbol{R}}. \tag{2.27}$$

Hence, the Wannier position operator defined by

$$\widehat{\boldsymbol{R}} := \sum_{\boldsymbol{R}\in\Lambda_R} \sum_{a=1}^{N} \widehat{W}^\dagger_{a;\boldsymbol{R}}\, \boldsymbol{R}\, \widehat{W}_{a;\boldsymbol{R}} \tag{2.28a}$$

is projected onto the lower bands by restricting the band index to the lower ones,

$$\begin{aligned} \widehat{\boldsymbol{X}}_R &:= \widehat{P}_{\widetilde{N}}\, \widehat{\boldsymbol{R}}\, \widehat{P}_{\widetilde{N}} \\ &= \sum_{\boldsymbol{R}\in\Lambda_R} \sum_{\tilde{a}=1}^{\widetilde{N}} \widehat{W}^\dagger_{\tilde{a};\boldsymbol{R}}\, \boldsymbol{R}\, \widehat{W}_{\tilde{a};\boldsymbol{R}}. \end{aligned} \tag{2.28b}$$

Hamiltonian (2.23a) in the Wannier basis is represented by

$$\widehat{H} = \sum_{\boldsymbol{R},\boldsymbol{R}'\in\Lambda_R} \sum_{a=1}^{N} \widehat{W}^{\dagger}_{a;\boldsymbol{R}}\, \mathcal{H}_{a;\boldsymbol{R}-\boldsymbol{R}'}\, \widehat{W}_{a;\boldsymbol{R}'}. \tag{2.29a}$$

The single-particle matrix elements,

$$\mathcal{H}_{a;\boldsymbol{R}-\boldsymbol{R}'} := \int\limits_{\Lambda^{\star}_{\mathrm{BZ}}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d}\, e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}\, \varepsilon_a(\boldsymbol{k}) \tag{2.29b}$$

may decay slower than exponentially with the separation $|\boldsymbol{R}-\boldsymbol{R}'|$ on the lattice Λ_R for some of the bands, i.e., locality in position space is not manifest in the Wannier basis.[60,61]

On the other hand, for any Hamiltonian describing the electronic band structure of crystalline phases of matter, there must exist a basis in which the Hamiltonian is local in position space, for electrons all originate from atomic orbitals. We can enforce locality of the Hamiltonian (2.23a) as follows. We shall assume that, for any momentum $\boldsymbol{k}$ from the Brillouin zone, there exists a unitary transformation from the band creation operators to the so-called orbital creation operators, i.e.,

$$\widehat{\psi}^{\dagger}_{\alpha}(\boldsymbol{k}) := \sum_{a=1}^{N} u^{(a)*}_{\alpha}(\boldsymbol{k})\, \widehat{\chi}^{\dagger}_{a}(\boldsymbol{k}) \tag{2.30a}$$

where we have reserved the greek index $\alpha = 1,\cdots,N$ for the orbital label. For any $\boldsymbol{k}$ from the Brillouin zone, the $N\times N$ matrix elements between the band $a=1,\cdots,N$ and orbital $\alpha=1,\cdots,N$ labels obey (i) the periodic boundary conditions

$$u^{(a)}_{\alpha}(\boldsymbol{k}) = u^{(a)}_{\alpha}\big(\boldsymbol{k}+(2\pi/\mathfrak{a})\,\boldsymbol{e}^{\mu}\big), \tag{2.30b}$$

for any $\mu=1,\cdots,d$, in order for $\widehat{\psi}_{\alpha}(\boldsymbol{k})$ to share with $\widehat{\chi}_{a}(\boldsymbol{k})$ the same twisted boundary condition (2.23d) and (ii) the orthonormality conditions

$$\sum_{\alpha=1}^{N} u^{(a)*}_{\alpha}(\boldsymbol{k})\, u^{(a')}_{\alpha}(\boldsymbol{k}) = \delta^{a,a'}, \qquad a,a'=1,\cdots,N, \tag{2.30c}$$

in order for the pair $\widehat{\psi}^{\dagger}_{\alpha}(\boldsymbol{k})$ and $\widehat{\psi}_{\alpha'}(\boldsymbol{k}')$ to share the same fermionic algebra (2.23c) as the pair $\widehat{\chi}^{\dagger}_{\alpha}(\boldsymbol{k})$ and $\widehat{\chi}_{\alpha'}(\boldsymbol{k}')$ does. Finally, we assume that the representation

$$\widehat{H} = \sum_{\boldsymbol{r},\boldsymbol{r}'\in\Lambda_r} \sum_{\alpha,\alpha'=1}^{N} \widehat{\psi}^{\dagger}_{\alpha;\boldsymbol{r}}\, \mathcal{H}_{\alpha,\alpha';\boldsymbol{r}-\boldsymbol{r}'}\, \widehat{\psi}_{\alpha';\boldsymbol{r}'} \tag{2.31a}$$

in terms of the Fourier transform

$$\widehat{\psi}^{\dagger}_{\alpha;\boldsymbol{r}} := \int\limits_{\Lambda^{\star}_{\mathrm{BZ}}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^{d/2}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\, \widehat{\psi}^{\dagger}_{\alpha}(\boldsymbol{k}), \tag{2.31b}$$

or, equivalently, the inverse Fourier transform

$$\widehat{\psi}^{\dagger}_{\alpha}(\boldsymbol{k}) =: \frac{1}{(2\pi/\mathfrak{a})^{d/2}} \sum_{\boldsymbol{r}\in\Lambda_r} e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\, \widehat{\psi}^{\dagger}_{\alpha;\boldsymbol{r}} \tag{2.31c}$$

for any orbital index $\alpha=1,\cdots,N$ and for any lattice point $\boldsymbol{r}=(r^{\mu})\in\Lambda_r$, has the single-particle matrix elements

$$\begin{aligned}\mathcal{H}_{\alpha,\alpha';\boldsymbol{r}-\boldsymbol{r}'} := \int\limits_{\Lambda^{\star}_{\mathrm{BZ}}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d}\, e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{r}-\boldsymbol{r}')} \\ \times \sum_{a=1}^{N} u^{(a)}_{\alpha}(\boldsymbol{k})\, \varepsilon_a(\boldsymbol{k})\, u^{(a)*}_{\alpha'}(\boldsymbol{k}),\end{aligned} \tag{2.31d}$$

that decay exponentially with increasing distance $|\boldsymbol{r}-\boldsymbol{r}'|$ for any pair of orbitals. Thus, locality on the lattice

$$\Lambda_r := \left\{ (r^{\mu})\in\mathbb{R}^d \,\middle|\, \frac{r^{\mu}}{\mathfrak{a}} = \theta^{\mu} \bmod 1,\ \mu=1,\cdots,d \right\} \tag{2.31e}$$

is manifest in the orbital basis. The lattices Λ_r and Λ_R share the same unit cell, however the two lattices can be shifted relative to each other in their embedding space $\mathbb{R}^d$ by any vector $\sum_{\mu=1}^{d} e_{\mu}\,\boldsymbol{e}^{\mu}$ with $-1\le e^{\mu}<1$ from their unit cell.

The projection operator (2.24) is not diagonal with respect to the orbital index while the projection operator (2.27) is neither diagonal with respect to the orbital index nor with respect to the lattice sites from Λ_r. Hence, the orbital position operator defined by

$$\widehat{\boldsymbol{r}} := \sum_{\boldsymbol{r}\in\Lambda_r} \sum_{\alpha=1}^{N} \widehat{\psi}^{\dagger}_{\alpha;\boldsymbol{r}}\, \boldsymbol{r}\, \widehat{\psi}_{\alpha;\boldsymbol{r}} \tag{2.32a}$$

turns after projection into (see Appendix A)

$$\begin{aligned}\widehat{\boldsymbol{X}}_r &:= \widehat{P}_{\widetilde{N}}\, \widehat{\boldsymbol{r}}\, \widehat{P}_{\widetilde{N}} \\ &= \sum_{\boldsymbol{R},\boldsymbol{R}'\in\Lambda_R} \sum_{\tilde{a},\tilde{a}'=1}^{\widetilde{N}} \widehat{W}^{\dagger}_{\tilde{a};\boldsymbol{R}}\, \boldsymbol{\mathcal{X}}_{\tilde{a},\tilde{a}';\boldsymbol{R},\boldsymbol{R}'}\, \widehat{W}_{\tilde{a}';\boldsymbol{R}'}\end{aligned} \tag{2.32b}$$

where we have introduced the single-particle kernel

$$\begin{aligned}\boldsymbol{\mathcal{X}}_{\tilde{a},\tilde{a}';\boldsymbol{R},\boldsymbol{R}'} := \int\limits_{\Lambda^{\star}_{\mathrm{BZ}}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d}\, e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} \\ \times \big[\delta_{\tilde{a},\tilde{a}'}\,\boldsymbol{R}' + \mathrm{i}\,\boldsymbol{A}_{\tilde{a}\tilde{a}'}(\boldsymbol{k})\big].\end{aligned} \tag{2.32c}$$

This kernel depends on the $U(\widetilde{N})$ gauge field $\boldsymbol{A}(\boldsymbol{k})$, an antihermitean $\widetilde{N}\times\widetilde{N}$ matrix whose components

$$\boldsymbol{A}_{\tilde{a}\tilde{a}'}(\boldsymbol{k}) := \sum_{\alpha=1}^{N} u^{(\tilde{a})*}_{\alpha}(\boldsymbol{k}) \left(\frac{\partial u^{(\tilde{a}')}_{\alpha}}{\partial\boldsymbol{k}}\right)(\boldsymbol{k}), \tag{2.32d}$$

are labeled by the lower band indices $\tilde{a},\tilde{a}'=1,\cdots,\widetilde{N}$ and obey periodic boundary conditions across the Brillouin zone.

The gauge field (2.32d) does not need to be a pure gauge as it originates from projecting the pure gauge field

$$\boldsymbol{A}_{aa'}(\boldsymbol{k}) := \sum_{\alpha=1}^{N} u_\alpha^{(a)*}(\boldsymbol{k}) \left(\frac{\partial u_\alpha^{(a')}}{\partial \boldsymbol{k}}\right)(\boldsymbol{k}) \tag{2.33}$$

by restricting the band indices $a, a' = 1, \cdots, N$ to the lower band indices $\tilde{a}, \tilde{a}' = 1, \cdots, \widetilde{N}$. Furthermore, the decomposition (2.30a) is not unique. Indeed, for any pair of orbital and band labels $\alpha, a = 1, \cdots, N$, the simultaneous transformations

$$u_\alpha^{(a)}(\boldsymbol{k}) =: \sum_{\mathsf{a}=1}^{N} u_\alpha^{(\mathsf{a})}(\boldsymbol{k})\, G_{\mathsf{a}a}^*(\boldsymbol{k}), \tag{2.34a}$$

on the one hand, and

$$\widehat{\chi}_a(\boldsymbol{k}) =: \sum_{\mathsf{a}=1}^{N} G_{a\mathsf{a}}(\boldsymbol{k})\, \widehat{\chi}_{\mathsf{a}}(\boldsymbol{k}), \tag{2.34b}$$

on the other hand, leaves $\widehat{\psi}_\alpha(\boldsymbol{k})$ unchanged. The $N \times N$ matrix $G(\boldsymbol{k})$ with the matrix elements $G_{a\mathsf{a}}(\boldsymbol{k})$ is unitary and obeys periodic boundary conditions across the Brillouin zone. The sans-serif font for the index $\mathsf{a} = 1, \cdots, N$ conveys that the vector $u^{(\mathsf{a})}(\boldsymbol{k})$ with the N components $u_\alpha^{(\mathsf{a})}(\boldsymbol{k})$ labeled by the orbitals $\alpha = 1, \cdots, N$ need not be anymore an eigenstate of the single-particle Bloch Hamiltonian.

Observe that for any triplet $a, \alpha, \mathsf{a} = 1, \cdots, N$, for any momentum $\boldsymbol{k}$ from the Brillouin zone, and any Cartesian unit vector $\boldsymbol{e}^\mu$ from $\mathbb{R}^d$, had we imposed the twisted boundary conditions

$$G_{a\mathsf{a}}\big(\boldsymbol{k} + (2\pi/\mathfrak{a})\boldsymbol{e}^\mu\big) = e^{-\mathrm{i}(2\pi\,\phi^\mu)}\; G_{a\mathsf{a}}(\boldsymbol{k}) \tag{2.35}$$

parametrized by the real numbers $0 \leq \phi^\mu < 1$ with $\mu = 1, \cdots, d$, it would then follow that

$$u_\alpha^{\mathsf{a}}\big(\boldsymbol{k} + (2\pi/\mathfrak{a})\, \boldsymbol{e}^\mu\big) = e^{-\mathrm{i}(2\pi\,\phi^\mu)}\, u_\alpha^{\mathsf{a}}(\boldsymbol{k}) \tag{2.36}$$

obeys twisted boundary conditions instead of periodic ones, while

$$\chi_{\mathsf{a}}\big(\boldsymbol{k} + (2\pi/\mathfrak{a})\, \boldsymbol{e}^\mu\big) = e^{+\mathrm{i}[2\pi\,(\theta^\mu + \phi^\mu)]}\, \chi_{\mathsf{a}}(\boldsymbol{k}) \tag{2.37}$$

obeys new twisted boundary conditions. As a corollary, the gauge field $\boldsymbol{A}_{\mathsf{a}\mathsf{a}'}$ obtained from Eq. (2.33) by substituting the band indices for the sans-serif ones would not be a pure gauge anymore as a result of this large gauge transformation. An example of a large gauge transformation is

$$G_{\boldsymbol{R}_0} = e^{+\mathrm{i}\,\widehat{\boldsymbol{P}}\cdot\boldsymbol{R}_0} \tag{2.38a}$$

for some $\boldsymbol{R}_0 \in \Lambda_R$ where $\widehat{\boldsymbol{P}}$ is the operator defined by the algebra

$$[\widehat{\boldsymbol{R}}, \widehat{\boldsymbol{P}}] = \mathrm{i}\,\widehat{Q} \tag{2.38b}$$

with $\widehat{Q}$ the fermion number operator. It acts on the single-particle states $|\chi^a(\boldsymbol{k})\rangle := \widehat{\chi}_a^\dagger(\boldsymbol{k})\,|0\rangle$, where $|0\rangle$ is the state annihilated by any band annihilation operator, by multiplication with the phase $e^{+\mathrm{i}\,\boldsymbol{k}\cdot\boldsymbol{R}_0}$. Thus, the action of the large gauge transformation (2.38) on $|\chi^a(\boldsymbol{k})\rangle$ is to change the boundary condition obeyed by $|\chi^a(\boldsymbol{k})\rangle$ from twisted to periodic. In turn, the large gauge transformation (2.38) acts on the single-particle states $|W_{\boldsymbol{R}}^a\rangle := \widehat{W}_{a;\boldsymbol{R}}^\dagger|0\rangle$ by shifting $\boldsymbol{R}$ to $\boldsymbol{R} - \boldsymbol{R}_0$, i.e., as a global translation of the lattice Λ_R.

Let the insulating noninteracting many-body ground state $|\Phi\rangle$ be obtained by filling all the single-particle states from the $\widetilde{N}$ bands below the spectral gap depicted in Fig. 1. The ground state $|\Phi\rangle$ is an $SU(\widetilde{N})$ singlet under the $U(\widetilde{N})$ gauge transformation defined by restricting the band index in Eq. (2.34b) to the subset of occupied band indices. Consequently, the ground state expectation value of any polynomial P of the components of the projected position operator $\widehat{\boldsymbol{X}}_r$ is, if it exists, invariant under the simultaneous $U(\widetilde{N})$ gauge transformation defined by restricting the band index in Eq. (2.34) to the subset of occupied band indices, i.e.,

$$\widehat{\chi}^\dagger(\boldsymbol{k}) \to \widehat{\chi}^\dagger(\boldsymbol{k})\, G^\dagger(\boldsymbol{k}), \qquad \widehat{\chi}(\boldsymbol{k}) \to G(\boldsymbol{k})\, \widehat{\chi}(\boldsymbol{k}), \tag{2.39a}$$

on the one hand, and

$$A_\mu(\boldsymbol{k}) \to G(\boldsymbol{k})\, A_\mu(\boldsymbol{k})\, G^\dagger(\boldsymbol{k}) - \big(\partial_\mu G\big)(\boldsymbol{k})\, G^\dagger(\boldsymbol{k}), \tag{2.39b}$$

on the other hand. Here, $G(\boldsymbol{k})$ is any unitary $\widetilde{N} \times \widetilde{N}$ matrix for any $\boldsymbol{k} \in \Lambda_{\mathrm{BZ}}^\star$, including one that changes the boundary conditions across the Brillouin zone, and matrix multiplication is implied in Eq. (2.39) with the operator-valued column-vectors $\widehat{\chi}(\boldsymbol{k})$ and row-vectors $\widehat{\chi}^\dagger(\boldsymbol{k})$ that have the components $\widehat{\chi}_{\tilde{a}}(\boldsymbol{k})$ and $\widehat{\chi}_{\tilde{a}}^\dagger(\boldsymbol{k})$, $\tilde{a} = 1, \cdots, \widetilde{N}$, respectively. Existence of $\langle\Phi|P(\widehat{\boldsymbol{X}}_r)|\Phi\rangle$ amounts to constructing a gauge-invariant regularization of $\langle\Phi|P(\widehat{\boldsymbol{X}}_r)|\Phi\rangle$. As we now prove, although not all polynomials P are compatible with a gauge-invariant regularization of $\langle\Phi|P(\widehat{\boldsymbol{X}}_r)|\Phi\rangle$, we do find polynomials P that admit such a gauge-invariant regularization.

To see this, we are going to momentarily dispense with complications arising from many-body terms and work solely in the single-particle Hilbert space. We define the pair of single-particle states

$$|W_{\boldsymbol{R}}^a\rangle := \widehat{W}_{a;\boldsymbol{R}}^\dagger\,|0\rangle, \qquad |\chi^a(\boldsymbol{k})\rangle := \widehat{\chi}_a^\dagger(\boldsymbol{k})\,|0\rangle, \tag{2.40a}$$

with $a = 1, \cdots, N$, $\boldsymbol{R} \in \Lambda_R$, $\boldsymbol{k} \in \Lambda_{\mathrm{BZ}}^\star$, and the pair of single-particle states

$$|\psi_{\boldsymbol{r}}^\alpha\rangle := \widehat{\psi}_{\alpha;\boldsymbol{r}}^\dagger\,|0\rangle, \qquad |\psi^\alpha(\boldsymbol{k})\rangle := \widehat{\psi}_\alpha^\dagger(\boldsymbol{k})\,|0\rangle, \tag{2.40b}$$

with $\alpha = 1, \cdots, N$ and $\boldsymbol{r} \in \Lambda_r$. The single-particle counterparts to the projected position operators (2.28b) and (2.32b) are defined to be

$$\widehat{\boldsymbol{X}}_R := \sum_{\boldsymbol{R}\in\Lambda_R} \sum_{\tilde{a}=1}^{\widetilde{N}} |W_{\boldsymbol{R}}^{\tilde{a}}\rangle\, \boldsymbol{R}\, \langle W_{\boldsymbol{R}}^{\tilde{a}}|, \tag{2.41a}$$

and, with the help of the single-particle kernel defined in Eq. (2.32c),

$$\widehat{\boldsymbol{X}}_r := \sum_{\boldsymbol{R},\boldsymbol{R}'\in\Lambda_R} \sum_{\tilde{a},\tilde{a}'=1}^{\widetilde{N}} |W^{\tilde{a}}_{\boldsymbol{R}}\rangle\, \boldsymbol{\mathcal{X}}_{\tilde{a},\tilde{a}';\boldsymbol{R},\boldsymbol{R}'}\, \langle W^{\tilde{a}'}_{\boldsymbol{R}'}|, \quad (2.41b)$$

respectively. Evidently, the trace over the (unprojected) single-particle Hilbert space of either $\widehat{\boldsymbol{X}}_R$ or $\widehat{\boldsymbol{X}}_r$ is ill-defined because of the ill-conditioned sum over the lattice Λ_R.

The situation is much better with the commutator between $\widehat{X}^\mu_r$ and $\widehat{X}^\nu_r$ for any $\mu,\nu = 1,\cdots,d$ owing to the identity

$$\left[\widehat{X}^\mu_r, \widehat{X}^\nu_r\right] = -\int\limits_{\Lambda^\star_{\rm BZ}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d}\, |\chi^{\tilde{a}}(\boldsymbol{k})\rangle F^{\tilde{a}\tilde{b}}_{\mu\nu}(\boldsymbol{k}) \langle\chi^{\tilde{b}}(\boldsymbol{k})| \quad (2.42a)$$

where the summation convention over the repeated band labels $\tilde{a},\tilde{b} = 1,\cdots,\widetilde{N}$ is implied and

$$F_{\mu\nu}(\boldsymbol{k}) := \left(\partial_\mu A_\nu\right)(\boldsymbol{k}) - \left(\partial_\nu A_\mu\right)(\boldsymbol{k}) + \left[A_\mu, A_\nu\right](\boldsymbol{k}). \quad (2.42b)$$

We refer the reader to Appendix A for the proof of Eq. (2.42). Evidently, the components of $\widehat{\boldsymbol{X}}_r$ are non-commutative if the non-Abelian gauge field $\boldsymbol{A}_\mu(\boldsymbol{k})$ has a nonvanishing field strength $\boldsymbol{F}_{\mu\nu}(\boldsymbol{k})$.[63] We can now safely take the trace of the commutator (2.42) over the single-particle Hilbert space,

$$\frac{1}{N_{\rm p}}\mathrm{Tr}\,\left[\widehat{X}^\mu_r, \widehat{X}^\nu_r\right] = -\frac{1}{\bar{\rho}}\int\limits_{\Lambda^\star_{\rm BZ}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d}\,\mathrm{tr}\,F_{\mu\nu}(\boldsymbol{k}) = -\frac{1}{\bar{\rho}}\int\limits_{\Lambda^\star_{\rm BZ}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d}\,\mathrm{tr}\,\left(\partial_\mu A_\nu - \partial_\nu A_\mu\right)(\boldsymbol{k}), \quad (2.43)$$

provided we multiply the functional trace Tr by the inverse of the total number of particles $N_{\rm p}$ in the insulating ground state $|\Phi\rangle$ to obtain an intensive quantity. Then, the ratio of the number of particles $N_{\rm p}$ to the single-particle Bloch wavefunction normalization constant is nothing but the average particle density $\bar{\rho}$. The symbol tr denotes the trace over the lower $\widetilde{N}$ bands. Equation (2.43) is well-defined and invariant under both pure and large gauge transformations of the form (2.39b).

For any integer $n = 2,3,\cdots$, we define the n-bracket of the n symbols $B_1, B_2, \cdots, B_n$ equipped with the product $\times$ to be their fully antisymmetrized product

$$[B_1, B_2, \cdots, B_n] \equiv \epsilon^{i_1 i_2 \cdots i_n} B_{i_1} \times B_{i_2} \times \cdots \times B_{i_n} \quad (2.44)$$

where the summation convention over repeated indices is implied and the symbol $\epsilon^{i_1 i_2 \cdots i_n}$ implies antisymmetrization. For convenience, we also introduce the terminology of the 1-bracket of the symbol B to be the symbol B itself.

Observe that any odd-bracket can be rewritten as

$$[B_1, B_2, \cdots, B_{2m+1}] = \left(\frac{1}{2}\right)^m \epsilon^{i_1 i_2 \cdots i_{2m+1}} \left[B_{i_1}, B_{i_2}\right] \times \cdots \times \left[B_{i_{2m-1}}, B_{i_{2m}}\right] \times B_{i_{2m+1}}, \quad (2.45a)$$

while any even-bracket can be rewritten as

$$[B_1, B_2, \cdots, B_{2m+2}] = \left(\frac{1}{2}\right)^{m+1} \epsilon^{i_1 i_2 \cdots i_{2m+2}} \left[B_{i_1}, B_{i_2}\right] \times \cdots \times \left[B_{i_{2m+1}}, B_{i_{2m+2}}\right] \quad (2.45b)$$

for $m = 0,1,2,\cdots$. For any integer $m = 0,1,2,\cdots$ such that $2m+2 \leq d$, it then follows that

$$\frac{1}{N_{\rm p}}\mathrm{Tr}\,\left[\widehat{X}^{\mu_1}_r, \cdots, \widehat{X}^{\mu_{2m+1}}_r, \widehat{X}^{\mu_{2m+2}}_r\right] = -\left(-\frac{1}{2}\right)^{m+1} \frac{1}{\bar{\rho}} \int\limits_{\Lambda^\star_{\rm BZ}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d}\, \epsilon^{i_1 \cdots i_{2m+1} i_{2m+2}}\, \mathrm{tr}\,\left(F_{i_1 i_2} \cdots F_{i_{2m+1} i_{2m+2}}\right)(\boldsymbol{k}) \quad (2.46)$$

with $i_1, \cdots, i_{2m+2} = \mu_1, \cdots, \mu_{2m+2}$. Equation (2.46) is well-defined and invariant under both pure and large gauge transformations of the form (2.39b). The right-hand side of Eq. (2.46) is proportional to the $(m+1)$-th Chern number.

For any integer n such that $2 \leq n \leq d$, the single-particle trace over any n-bracket of the components $\widehat{X}^{\mu_1}_R$,

$\cdots$, $\widehat{X}_R^{\mu_n}$ vanishes owing to the fact that (i) $\widehat{\boldsymbol{X}}_R$ is diagonal in the Wannier basis and (ii) performing the antisymmetrization $\epsilon_{i_1 i_2 \cdots i_n} R^{i_1} R^{i_2} \cdots R^{i_n} = 0$ before taking the sum over the lattice Λ_R.

In contrast to these brackets, neither is the single-particle trace over the 1-bracket of the component $\widehat{X}_r^\mu$ nor that of the 1-bracket of the component $\widehat{X}_R^\mu$ with $\mu = 1, \cdots, d$ well-defined. More generally, for any integer $m = 0, 1, 2, \cdots$ such that $2m + 1 \leq d$, the single-particle trace over any $(2m+1)$-bracket of the components $\widehat{X}_r^{\mu_1}$, $\cdots$, $\widehat{X}_r^{\mu_{2m+1}}$ is ill-defined because there always remain ill-conditioned sums over the lattice Λ_R. We are going to construct explicitly a suitable regularization of the single-particle trace over any $(2m+1)$-bracket of the components $\widehat{X}_r^{\mu_1}$, $\cdots$, $\widehat{X}_r^{\mu_{2m+1}}$ for $m = 0$ and $m = 1$ that can be nonvanishing and is invariant under any pure gauge transformation of the form (2.39b).

To this end, we need the important identity

$$\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R = \int\limits_{\Lambda_{\text{BZ}}^\star} \frac{\mathrm{d}^d \boldsymbol{k}}{(2\pi/\mathfrak{a})^d} \, |\chi^{\tilde{a}}(\boldsymbol{k})\rangle \, \mathrm{i} \, \boldsymbol{A}^{\tilde{a}\tilde{b}}(\boldsymbol{k}) \langle \chi^{\tilde{b}}(\boldsymbol{k})| \quad (2.47)$$

which is proved in Appendix A. We can now safely take the trace of Eq. (2.47) over the single-particle Hilbert space as we did in Eq. (2.43). We find

$$\frac{1}{N_{\text{p}}} \text{Tr} \left(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R \right) = \frac{\mathrm{i}}{\bar{\rho}} \int\limits_{\Lambda_{\text{BZ}}^\star} \frac{\mathrm{d}^d \boldsymbol{k}}{(2\pi/\mathfrak{a})^d} \, \text{tr} \, \boldsymbol{A}(\boldsymbol{k}). \quad (2.48)$$

Equation (2.48) is invariant under pure (but not large) gauge transformations of the form (2.39b). The loss of the invariance under the large gauge transformations of the form (2.39b) is to be attributed to the fact that the regularization (2.48) breaks translation invariance in that there are gauge nonequivalent ways of defining eigenstates of the projected position operator at short distances. In other words, it is not possible to construct a wave packet that can resolve distances smaller than the lattice spacing $\mathfrak{a}$. This fuzziness survives the limit $\mathfrak{a} \to 0$ as the breakdown of gauge symmetry under large gauge transformations of the form (2.39b).

The regularization (2.48) is not unique. For example, we could have chosen a regularization of the single-particle trace over any $(2m+1)$-bracket of the components $\widehat{X}_r^{\mu_1}$, $\cdots$, $\widehat{X}_r^{\mu_{2m+1}}$ that preserves this translation invariance through the heat kernel method.[64] The heat kernel regularization yields zero for all odd-brackets, a manifestly gauge invariant result! However, we reject this regularization because enforcing invariance under large gauge transformations of the form (2.39b) is not required by general symmetry arguments.

Yet another example of a regularization of the single-particle trace over any n-bracket of the components $\widehat{X}_r^{\mu_1}$, $\cdots$, $\widehat{X}_r^{\mu_n}$ is to do the replacement $\widehat{X}_r^{\mu_1} \to \widehat{X}_r^{\mu_1} - \widehat{X}_R^{\mu_1}$, $\cdots$, $\widehat{X}_r^{\mu_n} \to \widehat{X}_r^{\mu_n} - \widehat{X}_R^{\mu_n}$. With this substitution, the single-particle trace is well-defined, for it does not contain anymore ill-conditioned sums over the lattice Λ_R. However, whenever the single-particle trace over this n-bracket is nonvanishing, it breaks the invariance under pure $SU(\widetilde{N})$ gauge transformations of the form (2.39b) for any $n \geq 2$. For this reason, we reject this regularization.

We are now in position to state the main result of Sec. II A. When $d \geq 3$ and for any choice of the triplet $\mu_1, \mu_2, \mu_3 = 1, \cdots, d$, we define the regularized 3-bracket of the components $\widehat{X}_r^{\mu_1}$, $\widehat{X}_r^{\mu_2}$, and $\widehat{X}_r^{\mu_3}$ of the projected position operator (2.32b) to be[65,66]

$$\begin{aligned} 2 \left[\widehat{X}_r^{\mu_1}, \widehat{X}_r^{\mu_2}, \widehat{X}_r^{\mu_3} \right]_{\text{reg}} := & \left[\widehat{X}_r^{\mu_1}, \widehat{X}_r^{\mu_2}, \left(\widehat{X}_r^{\mu_3} - \widehat{X}_R^{\mu_3} \right) \right] + \left[\widehat{X}_r^{\mu_1}, \left(\widehat{X}_r^{\mu_2} - \widehat{X}_R^{\mu_2} \right), \widehat{X}_r^{\mu_3} \right] + \left[\left(\widehat{X}_r^{\mu_1} - \widehat{X}_R^{\mu_1} \right), \widehat{X}_r^{\mu_2}, \widehat{X}_r^{\mu_3} \right] \\ & - \left[\left(\widehat{X}_r^{\mu_1} - \widehat{X}_R^{\mu_1} \right), \left(\widehat{X}_r^{\mu_2} - \widehat{X}_R^{\mu_2} \right), \left(\widehat{X}_r^{\mu_3} - \widehat{X}_R^{\mu_3} \right) \right]. \end{aligned} \quad (2.49)$$

We have introduced the multiplicative factor 2 on the left-hand side in order to preserve the number of 3-brackets under regularization, namely one prior to regularization. Indeed, since we add 3-brackets that include one substitution $\boldsymbol{X}_r \to \boldsymbol{X}_r - \boldsymbol{X}_R$ and remove one 3-bracket that include 3 substitutions $\boldsymbol{X}_r \to \boldsymbol{X}_r - \boldsymbol{X}_R$ on the right-hand side, we are left with $3 - 1 = 2$ 3-brackets on the right-hand side. It is shown in Appendix A that we can safely take the single-particle trace over the regularized 3-bracket (2.49) after accounting for the same normalization as for the 1- and 2-brackets,

$$\frac{1}{N_{\text{p}}} \text{Tr} \left[\widehat{X}_r^{\mu_1}, \widehat{X}_r^{\mu_2}, \widehat{X}_r^{\mu_3} \right]_{\text{reg}} = -\frac{3}{4} \times \frac{\mathrm{i}}{\bar{\rho}} \int\limits_{\Lambda_{\text{BZ}}^\star} \frac{\mathrm{d}^d \boldsymbol{k}}{(2\pi/\mathfrak{a})^d} \, \epsilon^{i_1 i_2 i_3} \, \text{tr} \left(F_{i_1 i_2} \, A_{i_3} - \frac{2}{3} \, A_{i_1} \, A_{i_2} \, A_{i_3} \right) (\boldsymbol{k}) \quad (2.50)$$

where $i_1, i_2, i_3 = \mu_1, \mu_2, \mu_3$. As was the case with Eq. (2.48) and for the same reason, Eq. (2.50) is invariant under pure (but not large) gauge transformations of the form (2.39b).

The generalization to the case of any integer m such that $2m+1 \leq d$ consists in defining the regularized $(2m+$

1)-bracket $\left[\widehat{X}_r^{\mu_1},\widehat{X}_r^{\mu_2},\cdots,\widehat{X}_r^{\mu_{2m}},\widehat{X}_r^{\mu_{2m+1}}\right]_{\rm reg}$ by replacing the $(2m+1)$-bracket $\left[\widehat{X}_r^{\mu_1},\widehat{X}_r^{\mu_2},\cdots,\widehat{X}_r^{\mu_{2m}},\widehat{X}_r^{\mu_{2m+1}}\right]$ with the sum of all $(2m+1)$-brackets obtained by doing all the possible substitution $\widehat{X}_r^{\mu_i} \to \widehat{X}_r^{\mu_i} - \widehat{X}_R^{\mu_i}$ $(2l+1)$ times with $l=0,1,\cdots,m$ and adding all resulting $(2m+1)$-brackets weighted with the sign $(-)^l$. We then define a normal ordering by which all $\widehat{X}_r^{\mu_i}$ are placed to the left of all $\widehat{X}_r^{\mu_i} - \widehat{X}_R^{\mu_i}$ as if they were commuting numbers. Finally, we divide the resulting linear combination of $(2m+1)$-brackets by the integer equal to the absolute value of the alternating sum of the binomials coefficients $\begin{pmatrix} 2m+1 \\ 1 \end{pmatrix} - \begin{pmatrix} 2m+1 \\ 3 \end{pmatrix} \pm \cdots$. The single-particle trace over the regularized $(2m+1)$-bracket after accounting for the same normalization as for the even-brackets and the 1- and 3-brackets is intensive and proportional to the Chern-Simons invariant obtained from integrating over the d-dimensional Brillouin zone with $d \geq 2m+1$ the Chern-Simons $(2m+1)$ form.

It is time to draw a precise connection between the single-particle traces over the (regularized) brackets of the components of the position operator $\widehat{\boldsymbol{X}_r}$ and topological invariants.

We define the d Chern-Simons invariants built from Chern-Simons 1 forms in d-dimensional momentum space for any choice of $\mu = 1,\cdots,d$ as

$$\mathrm{CS}_{\mu}^{(1)} := \mathrm{i} \int \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi)^d} \,\mathrm{tr}\, A_{\mu}. \tag{2.51a}$$

We also define the $d(d-1)(d-2)/6$ Chern-Simons invariants built from Chern-Simons 3 forms in d-dimensional momentum space for any choice of $\mu,\mu,\lambda = 1,\cdots,d$ as

$$\mathrm{CS}_{\mu\nu\rho}^{(3)} := \frac{\epsilon^{IJK}}{4} \int \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi)^{d-1}} \,\mathrm{tr}\left(A_I F_{JK} - \frac{2}{3} A_I A_J A_K\right), \tag{2.51b}$$

where $I,J,K = \mu,\nu,\rho$. The integral on the right-hand side of Eq. (2.51a) and Eq. (2.51b) is quantized to half-integer values if the single-particle Hamiltonian obeys the chiral symmetry and the domain of integration is that of a d-dimensional torus T^d with the volume $(2\pi)^d$, i.e., $\mathfrak{a}=1$.[14] The 1D and 3D Chern-Simons invariants in d-dimensional momentum space carry the engineering dimensions of length raised to the powers $(1-d)$ and $(3-d)$, respectively. They are thus dimensionless if and only if $d=1$ and $d=3$, respectively.

The Chern-Simons invariants (2.51a) and (2.51b) are only well-defined modulo integer values under the $U(\widetilde{N})$ gauge transformations (2.39b) since the latter can change the former by their winding numbers, namely the numbers

$$\mathrm{i} \int \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi)^d} \,\mathrm{tr}\;\, G^{\dagger}\,\partial_{\mu} G, \qquad \mu = 1,\cdots,d, \tag{2.52a}$$

and

$$\frac{\mathrm{i}\epsilon^{IJK}}{6} \int \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi)^{d-1}} \,\mathrm{tr}\;\, \left[\left(G^{\dagger}\,\partial_I G\right)\left(G^{\dagger}\,\partial_J G\right)\left(G^{\dagger}\,\partial_K G\right)\right], \tag{2.52b}$$

with $I,J,K = \mu,\nu,\rho$ and $\mu,\nu,\rho = 1,\cdots,d$, respectively.

In contrast, the $d(d-1)/2$ first Chern numbers defined in d-dimensional momentum space as

$$\mathrm{Ch}_{\mu\nu}^{(1)} := \mathrm{i} \int \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi)^{d-1}} \,\mathrm{tr}\;\, F_{\mu\nu}, \qquad \mu,\nu = 1,\cdots,d, \tag{2.53}$$

can only take integer values if the domain of integration is that of a d-dimensional torus T^d with the volume $(2\pi)^d$ in momentum space,[67] irrespective of whether or not the single-particle Hamiltonian obeys the chiral symmetry. However, when chiral symmetry holds, the 1D Chern-Simons invariants (2.51a) are quantized.[19] Therefore, derivatives of these quantities vanish, which in turn implies that all first Chern numbers (2.53) vanish. Furthermore, the first Chern numbers (2.53) are invariant under the $U(\widetilde{N})$ gauge transformations (2.39b). The first Chern numbers defined in d-dimensional momentum space carry the engineering dimensions of $(2-d)$.

In closing, we reexpress our main result using second quantization and for the case of $d=3$ dimensions. We shall use the standard notation $:(\cdots):$ for normal ordering under which it is understood that creation operators are to be moved to the left of annihilation operators within the symbol $(\cdots)$ as if they were Grassman numbers. After identifying the single-particle states defined in Eq. (2.40a) with the single-particle holes resulting from annihilating a single-particle state from the insulating ground state $|\Phi\rangle$, we find that

$$\begin{aligned}\frac{1}{N_{\rm p}} \left\langle \Phi \middle| :\left[\widehat{X}_r^1,\widehat{X}_r^2,\widehat{X}_r^3\right]_{\rm reg}: \middle| \Phi \right\rangle = \\ - \frac{(2\pi)^2\mathrm{i}}{\bar{\rho}} \left[\frac{(2\pi)^3}{2} \frac{N_{\rm p}}{\bar{\rho}} \,\epsilon^{\mu\nu\rho}\,\mathrm{CS}_{\mu}^{(1)}\,\mathrm{Ch}_{\nu\rho}^{(1)} + 3\mathrm{CS}^{(3)}\right].\end{aligned} \tag{2.54}$$

Again, it should be noted that the right-hand side of Eq. (2.54) is entirely determined by its quantized topological numbers if the single-particle Hamiltonian obeys the chiral symmetry, and if the equality is understood modulo contributions from large $U(\widetilde{N})$ gauge transformations (2.39b) in which case

$$\frac{1}{N_{\rm p}} \left\langle \Phi \middle| :\left[\widehat{X}_r^1,\widehat{X}_r^2,\widehat{X}_r^3\right]_{\rm reg}: \middle| \Phi \right\rangle = -\frac{3(2\pi)^2\mathrm{i}}{\bar{\rho}} \,\mathrm{CS}^{(3)} \tag{2.55}$$

owing to $\mathrm{Ch}_{\nu\rho}^{(1)} = 0$ for any $\nu,\rho = 1,\cdots,d$.

B. Regularized 3-bracket and the Nambu bracket

On the one hand, we may define for any momentum $\boldsymbol{q}$ from the Brillouin zone the projected operator

$$\widehat{T}_R(\boldsymbol{q}) := e^{-\mathrm{i}\boldsymbol{q}\cdot\widehat{\boldsymbol{X}}_R} \tag{2.56}$$

with $\widehat{\boldsymbol{X}}_R$ defined in Eq. (2.41a) that acts on the single-particle Hilbert space defined in Eq. (2.40a). This operator is a projected translation operator in the Brillouin zone,

$$\widehat{T}_R(\boldsymbol{q})\,|\chi^a(\boldsymbol{k})\rangle = \sum_{\tilde{a}=1}^{\widetilde{N}} \delta^{a,\tilde{a}}\,|\chi^{\tilde{a}}(\boldsymbol{k}+\boldsymbol{q})\rangle \tag{2.57}$$

for any $a = 1, \cdots, N$. Its algebra under composition closes,

$$\widehat{T}_R(\boldsymbol{q}_1)\,\widehat{T}_R(\boldsymbol{q}_2) = \widehat{T}_R(\boldsymbol{q}_1+\boldsymbol{q}_2) \tag{2.58}$$

for any pair of momenta from the Brillouin zone.

On the other hand, we may also want to define for any momentum $\boldsymbol{q}$ from the Brillouin zone the projected operator

$$\widehat{T}_r(\boldsymbol{q}) := e^{-\mathrm{i}\boldsymbol{q}\cdot\widehat{\boldsymbol{X}}_r} \tag{2.59}$$

with $\widehat{\boldsymbol{X}}_r$ defined in Eq. (2.41b) that acts on the single-particle Hilbert space defined in Eq. (2.40b).

Be aware that $\widehat{T}_r(\boldsymbol{q})$ differs from the projection

$$\begin{aligned}\widehat{\rho}(\boldsymbol{q}) :=& \int\limits_{\Lambda^\star_{\mathrm{BZ}}} \frac{\mathrm{d}^d\boldsymbol{k}}{(2\pi/\mathfrak{a})^d} \sum_{\alpha=1}^{N}\sum_{\tilde{a},\tilde{a}'=1}^{\widetilde{N}} u_\alpha^{(\tilde{a})*}(\boldsymbol{k})\,u_\alpha^{(\tilde{a}')}(\boldsymbol{k}+\boldsymbol{q}) \\ &\times |\chi^{\tilde{a}}(\boldsymbol{k})\rangle\langle\chi^{\tilde{a}'}(\boldsymbol{k}+\boldsymbol{q})| \\ \equiv& \frac{1}{(2\pi/\mathfrak{a})^d}\,\widehat{P}_{\widetilde{N}}\,e^{-\mathrm{i}\boldsymbol{q}\cdot\widehat{\boldsymbol{r}}}\widehat{P}_{\widetilde{N}}\end{aligned} \tag{2.60a}$$

on the $\widetilde{N}$ lower bands of the momentum-resolved density operator $\widehat{\varrho}(\boldsymbol{q})$ defined through the Fourier expansion

$$\widehat{\varrho}_{\boldsymbol{r}} =: \int\limits_{\Lambda^\star_{\mathrm{BZ}}} \mathrm{d}^d\boldsymbol{q}\,e^{+\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}}\,\widehat{\varrho}(\boldsymbol{q}) \equiv \int\limits_{\Lambda^\star_{\mathrm{BZ}}} \frac{\mathrm{d}^d\boldsymbol{q}}{(2\pi/\mathfrak{a})^d}\,e^{+\mathrm{i}\boldsymbol{q}\cdot(\boldsymbol{r}-\widehat{\boldsymbol{r}})} \tag{2.60b}$$

of the unprojected density operator

$$\widehat{\varrho}_{\boldsymbol{r}} := \sum_{\alpha=1}^{N} |\psi^\alpha_{\boldsymbol{r}}\rangle\langle\psi^\alpha_{\boldsymbol{r}}| \tag{2.60c}$$

defined for any site $\boldsymbol{r}$ of lattice Λ_r.

The task of computing the regularized n-bracket of the operators $\widehat{T}_r(\boldsymbol{q}_1), \cdots, \widehat{T}_r(\boldsymbol{q}_n)$ is formidable for arbitrary momenta $\boldsymbol{q}_1, \cdots, \boldsymbol{q}_n$ from the Brillouin zone. However, an expansion in the momenta up to order n is feasible in the limit of small momenta. We undertake such an expansion for the 3-bracket with the help of the (classical) Nambu bracket.

To simplify notation, we work with $d = 3$. Let $f_i(\boldsymbol{x})$ with $i = 1, 2, 3$ denote three functions with the Taylor expansions

$$f_i(\boldsymbol{x}) = f_i(\boldsymbol{0}) + \sum_{\mu=1}^{3} \left(\partial_\mu f_i\right)(\boldsymbol{0})\,x^\mu + \cdots \tag{2.61}$$

at the origin of $\boldsymbol{x} \in \mathbb{R}^3$. For any pair of functions f_1 and f_2, or for any triplet of functions f_1, f_2, and f_3 their classical Poisson and Nambu brackets were defined in Eqs. (2.10b) and (2.16b), respectively. For any pairs $\mu, \nu = 1, 2, 3$ and f_i, f_j, with $i, j = 1, 2, 3$, we shall also need the variant

$$\left\{f_i, f_j\right\}^{\mu\nu}_{\mathrm{P}}(\boldsymbol{0}) := \sum_{I,J=\mu,\nu} \epsilon_{IJ}\left(\partial^I f_i\right)\left(\partial^J f_j\right)(\boldsymbol{0}) \tag{2.62}$$

of the Poisson bracket, respectively. From the operator identity (A76) follows that the single-particle trace over the regularized 3-bracket of $f_1(\widehat{\boldsymbol{X}})$, $f_2(\widehat{\boldsymbol{X}})$, and $f_3(\widehat{\boldsymbol{X}})$ admits the Taylor expansion

$$\mathrm{Tr}\,\left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]_{\mathrm{reg}} = \epsilon^{ijk}\,f_i\,\left\{f_j, f_k\right\}^{\mu\nu}_{\mathrm{P}}(\boldsymbol{0})\,\mathrm{Tr}\,\left[\widehat{X}^\mu_r, \widehat{X}^\nu_r\right] + \{f_1, f_2, f_3\}_{\mathrm{N}}(\boldsymbol{0})\,\mathrm{Tr}\,\left[\widehat{X}^1_r, \widehat{X}^2_r, \widehat{X}^3_r\right]_{\mathrm{reg}} + \cdots . \tag{2.63}$$

(A summation convention is implied over the repeated indices $\mu, \nu = 1, 2, 3$ and $i, j, k = 1, 2, 3$ on the right-hand side.) This expansion preserves the invariance under the pure gauge transformations of the form (2.39b). Moreover, in the chiral class,

$$\mathrm{Tr}\,\left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]_{\mathrm{reg}} = \{f_1, f_2, f_3\}_{\mathrm{N}}(\boldsymbol{0})\,\mathrm{Tr}\,\left[\widehat{X}^1_r, \widehat{X}^2_r, \widehat{X}^3_r\right]_{\mathrm{reg}} + \cdots \tag{2.64}$$

and

$$\mathrm{Tr}\,\left[\widehat{T}_r(\boldsymbol{q}_1), \widehat{T}_r(\boldsymbol{q}_2), \widehat{T}_r(\boldsymbol{q}_3)\right]_{\mathrm{reg}} = +\,\mathrm{i}\,(\boldsymbol{q}_1 \wedge \boldsymbol{q}_2)\cdot\boldsymbol{q}_3\,\mathrm{Tr}\,\left[\widehat{X}^1_r, \widehat{X}^2_r, \widehat{X}^3_r\right]_{\mathrm{reg}} + \cdots . \tag{2.65}$$

Equation (2.64) admits the following interpretation. The functions f_1, f_2, and f_3 may represent a coordinate transformation in 3D space. If this transformation preserves volume, its Jacobian, i.e., the Nambu bracket, equals 1. If chiral symmetry holds, the trace over the regularized 3-bracket of the projected position operator $\widehat{\boldsymbol{X}}_r$ is to lowest order in the Taylor expansion invariant under volume preserving diffeomorphisms, while quantum corrections appear at higher order.

Had we restricted ourselfs to $d = 2$, the transformation property of the 2-bracket (commutator) under the smooth coordinate transformation

$$(x^1, x^2) \to \Big(f_1(\boldsymbol{x}), f_2(\boldsymbol{x})\Big), \qquad \boldsymbol{x} \equiv (x^1, x^2) \in \mathbb{R}^2, \tag{2.66}$$

is

$$\Big[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r)\Big] = \{f_1, f_2\}_{\rm P}(\boldsymbol{0}) \, \Big[\widehat{X}_r^1, \widehat{X}_r^2\Big] + \cdots . \tag{2.67}$$

Except for the quantum corrections contained in $\cdots$, the 2-bracket of the projected position operator $\widehat{\boldsymbol{X}}_r$ is thus invariant under area-preserving diffeomorphisms. The difference between the 2-bracket and the regularized 3-bracket is, according to Eq. (A76), that for the latter it is necessary to invoke chiral symmetry and taking the single-particle trace in order to guarantee invariance under volume-preserving diffeomorphisms.

The algebra obeyed by the set of diffeomorphisms of the Euclidean plane that leave the Poisson bracket invariant realizes the so-called classical w_∞ algebra. Thus, Eq. (2.67) draws the connection to a quantum version of the w_∞ algebra. For the quantum Hall effect the relevant quantum version is the W_∞ algebra (see Refs. 45, 46, 47, and 48) obeyed by the projected density operators in a Landau level.[33,35–37] A manifestation of the connection between the w_∞ and W_∞ algebras is found in the nondissipative Hall viscosity, which can be viewed as the response function of the quantum fluid to an infinitesimal area-preserving deformation.[68] In turn, an incompressible 2D classical fluid may be described in terms of a one-form gauge field, as appears in the Chern-Simons theory relevant to the quantum Hall effect (QHE).[69–71]

In 3D and for Bloch Hamiltonians belonging to the chiral symmetry class, the invariance under volume-preserving diffeomorphisms of 3D Euclidean space displayed in Eq. (2.64) to lowest order in the Taylor expansion draws a similiar connection to a quantum algebra that generalizes the classical algebra obeyed by volume-preserving diffeomorphisms. In the description of ideal 3D classical fluids a two-form gauge field naturally arises as a consequence of volume preserving diffeomorphisms.[72] Such a two-form gauge field also appears in the 3D BF theory that is believed to be relevant to 3D topological insulators.[73]

C. Massive Dirac fermions

In Sec. II A, we have related the ground state expectation values of the commutator and of the regularized 3-bracket of the projected position operators $\widehat{\boldsymbol{X}}_r$ to quantized topological numbers, namely the Chern numbers and Chern-Simons invariants. By contrast, we have recalled in Eq. (2.4b) that a Landau level has the special property that the commutator of projected position operators *itself* is nothing but an imaginary number

$$\begin{aligned}[\widehat{X}^\mu, \widehat{X}^\nu] &= -F_{\mu\nu} \\ &= \mathrm{i}\,\epsilon_{\mu\nu}\,\ell_B^2\end{aligned} \tag{2.68}$$

where $\mu, \nu = 1, 2$. In other words, the Berry curvature is constant in a Landau level.

Here, we are going to show that the same is true for massive Dirac electrons in 2D, if the limit of small momenta $\boldsymbol{k} \to 0$ is considered. We then extend the discussion to massive Dirac electrons in 3D, where we consider the 3-bracket of projected position operators in the same limit of small momenta.

In 2D Euclidean flat space, a single flavor of Dirac fermions with mass m and in the fundamental representation of the Lorentz group is governed by the single-particle Hamiltonian in momentum space

$$\mathcal{H}_{\rm 2D}(\boldsymbol{k}) := k_1\sigma_1 + k_2\sigma_2 + m\sigma_3. \tag{2.69}$$

As usual, we use σ_0 for the 2×2 unit matrix, while σ_1, σ_2, and σ_3 are the three Pauli matrices.

This Hamiltonian supports two bands with the Bloch states $|\chi^\pm(\boldsymbol{k})\rangle$, the nondegenerate energy eigenvalues

$$\varepsilon^{(\pm)}(\boldsymbol{k}) = \pm\sqrt{\boldsymbol{k}^2 + m^2}, \tag{2.70}$$

and the Berry curvatures

$$F_{\mu\nu}^{(\pm)}(\boldsymbol{k}) = \mathrm{i}\,\epsilon_{\mu\nu}\,\frac{m}{2\left[\varepsilon^{(\pm)}(\boldsymbol{k})\right]^3}, \tag{2.71}$$

for $\mu, \nu = 1, 2$. Upon projection to the lower band $\varepsilon^{(-)}(\boldsymbol{k})$, we can combine Eq. (2.42a) with Eq. (2.71) to deduce that

$$\begin{aligned}\langle\chi^-(\boldsymbol{k})|[\widehat{X}_r^\mu, \widehat{X}_r^\nu]|\chi^-(\boldsymbol{k})\rangle &= -F_{\mu\nu}^{(-)}(\boldsymbol{k}) \\ &= \mathrm{i}\,\epsilon_{\mu\nu}\,\ell_{\rm D}^2\,\mathrm{sgn}\,m + \mathcal{O}(\boldsymbol{k}^2)\end{aligned} \tag{2.72a}$$

for $\mu, \nu = 1, 2$. The Dirac counterpart to the magnetic length in the QHE is here

$$\ell_{\rm D} := \frac{1}{\sqrt{2}\,m}. \tag{2.72b}$$

As announced, the algebra (2.72) reproduces the algebra (2.68) in the limit $\boldsymbol{k} \to 0$. The first Chern number of the lower band is given by

$$\begin{aligned}\mathrm{Ch}^{(1)} &:= \frac{\mathrm{i}}{2\pi}\int\limits_{\mathbb{R}^2} \mathrm{d}^2\boldsymbol{k}\,\mathrm{tr}\,F_{12}^{(-)} \\ &= \frac{\mathrm{sgn}\,m}{2}.\end{aligned} \tag{2.73}$$

In 3D Euclidean flat space, a single flavor of Dirac fermions with mass m and in the fundamental representation of the Lorentz group is governed by the single-particle Hamiltonian in momentum space

$$\mathcal{H}_{\rm 3D}(\boldsymbol{k}) := \sum_{\mu=1}^{3} k_\mu \alpha_\mu - {\rm i} m \beta \gamma_5, \tag{2.74a}$$

where we have defined the Hermitian 4×4 matrices

$$\alpha_\mu = \begin{pmatrix} 0 & \sigma_\mu \\ \sigma_\mu & 0 \end{pmatrix}, \quad \beta = \begin{pmatrix} \sigma_0 & 0 \\ 0 & -\sigma_0 \end{pmatrix}, \quad \gamma_5 = \begin{pmatrix} 0 & \sigma_0 \\ \sigma_0 & 0 \end{pmatrix}. \tag{2.74b}$$

Observe that this Hamiltonian has the chiral symmetry

$$\gamma_5 \, \mathcal{H}_{\rm 3D}(\boldsymbol{k}) \, \gamma_5 = - \mathcal{H}_{\rm 3D}(\boldsymbol{k}) \tag{2.75}$$

for all $\boldsymbol{k} \in \mathbb{R}^3$. The spectrum of Hamiltonian (2.74a) consists of two doubly degenerate bands with the Bloch states $|\chi^{\pm,a}(\boldsymbol{k})\rangle$, the energy eigenvalues

$$\varepsilon^{(\pm)}(\boldsymbol{k}) = \pm \sqrt{\boldsymbol{k}^2 + m^2}, \tag{2.76}$$

and the non-Abelian Berry field strengths

$$F^{(\pm)}_{\mu\nu}(\boldsymbol{k}) = \pm {\rm i} \, \ell_{\rm D}^2 \, \epsilon_{\mu\nu\lambda} \, \gamma^\lambda + \mathcal{O}(|\boldsymbol{k}|) \tag{2.77}$$

for $\mu, \nu = 1, 2, 3$, where $\boldsymbol{\gamma}^{\sf T} = (-\sigma_1, \sigma_2, \sigma_3)$. Upon projection to the lower band $\varepsilon^{(-)}(\boldsymbol{k})$, we can combine Eq. (2.42a) with Eq. (2.77) to deduce that

$$\mathrm{tr} \left(\langle \chi^{-,a}(\boldsymbol{k}) | [\widehat{X}^\mu_r, \widehat{X}^\nu_r] | \chi^{-,b}(\boldsymbol{k}) \rangle \right) = 0 + \mathcal{O}(|\boldsymbol{k}|) \tag{2.78}$$

for $\mu, \nu = 1, 2, 3$, as expected for a system with chiral symmetry. In contrast, Eq. (2.50) delivers

$$\mathrm{tr} \left(\langle \chi^{-,a}(\boldsymbol{k}) | [\widehat{X}^1_r, \widehat{X}^2_r, \widehat{X}^3_r]_{\rm reg} | \chi^{-,b}(\boldsymbol{k}) \rangle \right) = {\rm i} \, 3 \sqrt{2} \, \ell_{\rm D}^3 + \mathcal{O}(|\boldsymbol{k}|). \tag{2.79}$$

The definition (2.72b) of $\ell_{\rm D}$ has carried over.

D. Operator product expansions for the projected single-particle density operators

Until now, we have considered the noncommutative relations obeyed by the projected position operator assuming translation invariance in Euclidean flat spaces. This noncommutative geometry encodes topological properties of the noninteracting many-body ground state in view of the expectation values (2.43), (2.48), and (2.50). Moreover, according to Eq. (2.32), it is also predicated on some underlying noncommutative relations obeyed by the second-quantized fermion density operator projected onto the occupied bands of the insulating ground state.

On the other hand, GMP were able to derive for the 2D QHE the closed algebra obeyed by the single-particle electronic density projected onto the lowest Landau level. Can we do the same for the single-particle fermionic density projected onto one band, say, of a 3D topological band insulator?

To answer this question, we resort to a tight-binding model defined on a lattice Λ with a Brillouin zone BZ, and on which we impose periodic boundary conditions. We assume, without loss of generality, that the lattice is three dimensional. In this spirit, we turn our attention to the single-particle electronic density defined on a given site $\boldsymbol{r}$ of a lattice Λ as

$$\widehat{\varrho}_{\boldsymbol{r}} := \sum_{\alpha=1}^{N} |\boldsymbol{r}, \alpha\rangle\langle \boldsymbol{r}, \alpha|, \tag{2.80a}$$

where $\alpha = 1, \cdots, N$ labels degrees of freedom on every lattice site, e.g., spin or orbitals. These operators obey the closed algebra

$$\widehat{\varrho}_{\boldsymbol{r}_1} \, \widehat{\varrho}_{\boldsymbol{r}_2} = \delta_{\boldsymbol{r}_1, \boldsymbol{r}_2} \, \widehat{\varrho}_{\boldsymbol{r}_1} \tag{2.80b}$$

owing to the orthonormality of the single-particle states

$$\langle \boldsymbol{r}_1, \alpha_1 | \boldsymbol{r}_2, \alpha_2 \rangle = \delta_{\boldsymbol{r}_1, \boldsymbol{r}_2} \, \delta_{\alpha_1, \alpha_2} \tag{2.80c}$$

for any pair of sites $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ from the lattice Λ and for any pair of orbitals $\alpha_1, \alpha_2 = 1, \cdots N$. As a consequence, these operators commute pairwise.

The Fourier transform of $\widehat{\varrho}_{\boldsymbol{r}}$ in terms of the orthonormal Bloch states $|\boldsymbol{k}, \alpha\rangle$ labeled by the momentum $\boldsymbol{k}$ from the BZ and orbital index $\alpha = 1, \cdots, N$ reads

$$\widehat{\varrho}_{\boldsymbol{q}} = \sum_{\boldsymbol{k} \in {\rm BZ}} \sum_{\alpha=1}^{N} |\boldsymbol{k}, \alpha\rangle\langle \boldsymbol{k} + \boldsymbol{q}, \alpha| \tag{2.81a}$$

for any $\boldsymbol{q} \in$ BZ. These operators obey the closed algebra

$$\widehat{\varrho}_{\boldsymbol{q}_1} \, \widehat{\varrho}_{\boldsymbol{q}_2} = \widehat{\varrho}_{\boldsymbol{q}_1 + \boldsymbol{q}_2}, \tag{2.81b}$$

owing to the orthonormality of the single-particle states

$$\langle \boldsymbol{q}_1, \alpha_1 | \boldsymbol{q}_2, \alpha_2 \rangle = \delta_{\boldsymbol{q}_1, \boldsymbol{q}_2} \, \delta_{\alpha_1, \alpha_2} \tag{2.81c}$$

for any pair of momentum $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$ from the BZ and for any pair of orbitals $\alpha_1, \alpha_2 = 1, \cdots N$. As a consequence, these operators commute pairwise.

Consider now a basis transformation in the α degrees of freedom for every $\boldsymbol{k} \in$ BZ that is parametrized by the $N \times N$ complex-valued numbers $u^{(b)}_{\boldsymbol{k}, \alpha}$ with $\alpha, b = 1, \cdots, N$, i.e.,

$$\left| u^{(b)}_{\boldsymbol{k}} \right\rangle := \sum_{\alpha=1}^{N} u^{(b)}_{\boldsymbol{k}, \alpha} |\boldsymbol{k}, \alpha\rangle, \qquad b = 1, \cdots, N. \tag{2.82}$$

The ket $|u_{\boldsymbol{k}}, b\rangle$ labeled by $\boldsymbol{k} \in$ BZ for any given $b = 1, \cdots, N$ should be thought of as Bloch state of the b-th band of a single-particle Hamiltonian. This Hamiltonian shares the translational symmetry of Λ and periodic boundary conditions are imposed. For any $\boldsymbol{q} \in$ BZ, we

define the density operator projected on a single (nondegenerate) band $\tilde{b}$ by

$$\widehat{\rho}_{\boldsymbol{q}} := \sum_{\boldsymbol{k}\in \mathrm{BZ}} \sum_{\alpha=1}^{N} u^{(\tilde{b})*}_{\boldsymbol{k},\alpha} u^{(\tilde{b})}_{\boldsymbol{k}+\boldsymbol{q},\alpha} \left|u^{(\tilde{b})}_{\boldsymbol{k}}\right\rangle \left\langle u^{(\tilde{b})}_{\boldsymbol{k}+\boldsymbol{q}}\right|. \tag{2.83}$$

The projected operators $\widehat{\rho}_{\boldsymbol{q}}$ with $\boldsymbol{q} \in \mathrm{BZ}$ are invariant under the simultaneous local U(1) gauge transformations defined by

$$u^{(\tilde{b})}_{\boldsymbol{k},\alpha} \to e^{\mathrm{i}\varphi_{\boldsymbol{k}}} u^{(\tilde{b})}_{\boldsymbol{k},\alpha} \tag{2.84a}$$

on the one hand, and

$$\left|u^{(\tilde{b})}_{\boldsymbol{k}}\right\rangle \to e^{\mathrm{i}\varphi_{\boldsymbol{k}}} \left|u^{(\tilde{b})}_{\boldsymbol{k}}\right\rangle \tag{2.84b}$$

on the other hand, for all $\alpha = 1, \cdots, N$, $\boldsymbol{k} \in \mathrm{BZ}$, and any real-valued function $\varphi_{\boldsymbol{k}}$. They do not obey anymore the algebra (2.81b). In the long-wavelength limit $\boldsymbol{q}_1, \boldsymbol{q}_2 \ll 1$ (the lattice spacing of Λ is set to unity), their commutation relation is [38–40]

$$\left[\widehat{\rho}_{\boldsymbol{q}_1}, \widehat{\rho}_{\boldsymbol{q}_2}\right] = q_1^{\mu} q_2^{\nu} \sum_{\boldsymbol{k}\in \mathrm{BZ}} F_{\mu\nu,\boldsymbol{k}} \left|u^{(\tilde{b})}_{\boldsymbol{k}}\right\rangle \left\langle u^{(\tilde{b})}_{\boldsymbol{k}+\boldsymbol{q}_1+\boldsymbol{q}_2}\right| \tag{2.85a}$$

to leading order in an expansion in powers of the components of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$, where

$$F_{\mu\nu,\boldsymbol{k}} := \partial_{\mu} A_{\nu,\boldsymbol{k}} - \partial_{\nu} A_{\mu,\boldsymbol{k}} \tag{2.85b}$$

and

$$A_{\mu,\boldsymbol{k}} := \sum_{\alpha=1}^{N} u^{(\tilde{b})*}_{\boldsymbol{k},\alpha} \, \partial_{\mu} u^{(\tilde{b})}_{\boldsymbol{k},\alpha} \tag{2.85c}$$

for $\mu, \nu = 1, 2, 3$ are the Abelian Berry curvature and the Abelian Berry connection, respectively, and ∂_{μ} is understood as the derivative with respect to the momentum component k^{μ}. The operator product expansion (2.85a) closes only if $F_{\mu\nu,\boldsymbol{k}}$ is *independent* of $\boldsymbol{k}$, in which case

$$\left[\widehat{\rho}_{\boldsymbol{q}_1}, \widehat{\rho}_{\boldsymbol{q}_2}\right] = -\frac{\mathrm{i}}{2\pi} \left(\boldsymbol{q}_1 \wedge \boldsymbol{q}_2\right) \cdot \mathbf{Ch} \; \widehat{\rho}_{\boldsymbol{q}_1+\boldsymbol{q}_2} \tag{2.86a}$$

to leading order in an expansion in powers of the components of $\boldsymbol{q}_1$ and $\boldsymbol{q}_2$, where

$$\mathrm{Ch}^{\lambda} := \frac{2\pi\mathrm{i}}{L^3} \frac{\epsilon^{\mu\nu\lambda}}{2} \sum_{\boldsymbol{k}\in \mathrm{BZ}} F_{\mu\nu,\boldsymbol{k}} \tag{2.86b}$$

with $\lambda = 1, 2, 3$ are the components of the vector $\mathbf{Ch}$ made of the three first Chern numbers characterizing any nondegenerate band in 3D space.[74] (A summation convention is implied for the repeated indices $\mu, \nu = 1, 2, 3$.) In the thermodynamic limit by which the linear size L over which the periodic boundary conditions are imposed is taken to infinity or, equivalently, the lattice spacing is taken to zero, each first Chern number is quantized.

The IQHE is an example in 2D for which the condition of constant Berry curvature $F_{\mu\nu,\boldsymbol{k}}$ is met. In this context, the closed operator product expansion (2.86a) was found by GMP (in fact, the operator product expansion for the projected density operators closes to all orders in $\boldsymbol{q}$ in this case, and thus delivers a closed algebra for the projected density operators).[33] With the help of this algebra, GMP argue, within a single-mode approximation, that FQH states are incompressible.

Recently, it was shown that lattice models with flat bands and nonzero Chern number also support incompressible FQH ground states,[50–53] even though their Berry curvature is not constant over the BZ. This result suggests to approximate the commutator (2.85a) by the closed algebra (2.86a), that is, to replace $F_{\mu\nu,\boldsymbol{k}}$ with its average value over the BZ.[38,39]

We will now consider the 3-bracket of three projected density operators, and expand it to third order in the momenta

$$\begin{aligned}\left[\widehat{\rho}_{\boldsymbol{q}_1}, \widehat{\rho}_{\boldsymbol{q}_2}, \widehat{\rho}_{\boldsymbol{q}_3}\right] = \epsilon^{ijk} \frac{1}{2} \sum_{\boldsymbol{k}\in \mathrm{BZ}} \Bigg\{ & q_i^{\mu} q_j^{\nu} F_{\mu\nu,\boldsymbol{k}} + q_i^{\mu} q_j^{\nu} q_k^{\lambda} F_{\mu\nu,\boldsymbol{k}} A_{\lambda,\boldsymbol{k}} \\ & + q_i^{\mu} q_j^{\nu} q_j^{\lambda} \left[\partial_{\mu} \left(\sum_{\alpha=1}^{N} u^{(\tilde{b})*}_{\boldsymbol{k},\alpha} \, \partial_{\nu}\partial_{\lambda} u^{(\tilde{b})}_{\boldsymbol{k},\alpha}\right) - \left(\partial_{\nu} + 2A_{\nu}\right) \partial_{\lambda} A_{\mu}\right] \Bigg\} \left|u^{(\tilde{b})}_{\boldsymbol{k}}\right\rangle \left\langle u^{(\tilde{b})}_{\boldsymbol{k}+\boldsymbol{q}_1+\boldsymbol{q}_2+\boldsymbol{q}_3}\right|,\end{aligned} \tag{2.87}$$

where the summation convention over the repeated indices $i, j, k = 1, 2, 3$ and $\mu, \nu, \lambda = 1, 2, 3$ is implied. Equation (2.87) is invariant under the local gauge transformation (2.84), up to contributions of fourth order in $\boldsymbol{q}$. The term of second order in $\boldsymbol{q}$ comes multiplied by the Berry curvature, i.e., the density associated with the topological invariants Ch^{λ} for $\lambda = 1, 2, 3$ defined in Eq. (2.86b). As for the second term on the right-hand side, we recognize the integrand of the Abelian Chern-Simons form.

The term that dominates the 3-bracket of projected density operators at long wavelength is thus not equal to the 3-bracket of the position operator $\widehat{\boldsymbol{X}}_r$. According to Eq. (2.50), the latter was determined by the Chern-Simons 3 form and not by the Chern number density.

This stands in contrast to the long wavelength limit of the 2-bracket (commutator) of projected density operators which coincides with the 2-bracket of position operators. However, the connection between the projected density and position operators is recovered on the level of the 3-brackets, if one considers the derivative of the density operator with respect to momentum instead. This choice is motivated by the fact that the Fourier components of the density operator in momentum space are the generators of translations in momentum space [recall Eq. (2.60)]. Indeed, it follows from Eq. (2.87) that

$$\begin{aligned}\Big[\partial_{q_1^\alpha}\widehat{\rho}_{\boldsymbol{q}_1},\partial_{q_2^\beta}\widehat{\rho}_{\boldsymbol{q}_2},\partial_{q_3^\gamma}\widehat{\rho}_{\boldsymbol{q}_3}\Big]\\ =\frac{\epsilon^{\alpha\beta\gamma}}{2}\sum_{\boldsymbol{k}\in\mathrm{BZ}}\epsilon^{\mu\nu\lambda}A_{\mu,\boldsymbol{k}}F_{\nu\lambda,\boldsymbol{k}}\left|u^{(\tilde{b})}_{\boldsymbol{k}}\right\rangle\left\langle u^{(\tilde{b})}_{\boldsymbol{k}+\boldsymbol{q}_1+\boldsymbol{q}_2+\boldsymbol{q}_3}\right|\end{aligned} \tag{2.88a}$$

holds to lowest order in the momenta $\boldsymbol{q}_1$, $\boldsymbol{q}_2$ and $\boldsymbol{q}_2$ and is thus determined by the Chern-Simons 3-form (the Chern-Simons density in 3D). We define its average over the BZ to be

$$\theta:=\frac{\pi^2}{L^3}\sum_{\boldsymbol{k}\in\mathrm{BZ}}\epsilon^{\mu\nu\lambda}\,F_{\mu\nu,\boldsymbol{k}}\,A_{\lambda,\boldsymbol{k}}, \tag{2.88b}$$

which is only invariant under the local gauge transformations (2.84a) that leave the boundary conditions in the BZ unchanged. If the Chern-Simons density is nearly constant and thus independent of $\boldsymbol{k}$ in the entire BZ, we may approximate Eq. (2.88a) by

$$\Big[\partial_{q_1^\alpha}\widehat{\rho}_{\boldsymbol{q}_1},\partial_{q_2^\beta}\widehat{\rho}_{\boldsymbol{q}_2},\partial_{q_3^\gamma}\widehat{\rho}_{\boldsymbol{q}_3}\Big]\approx\epsilon_{\alpha\beta\gamma}\frac{\mathfrak{a}^3\,\theta}{2\pi^2}\,\widehat{\rho}_{\boldsymbol{q}_1+\boldsymbol{q}_2+\boldsymbol{q}_3}, \tag{2.88c}$$

where $\mathfrak{a}$ is the lattice spacing.

Insulators for which the invariants Ch^λ with $\lambda=1,2,3$ are nonvanishing can be viewed as a 3D extension of an IQHE or a layered system of 2D Chern insulators. In this case, Ch^λ with $\lambda=1,2,3$ parametrizes the quantized off-diagonal part of the conductivity tensor.[74] The physics of such insulators is not intrinsically 3D and they are thus not our primary interest here.

Even if the Berry curvature vanishes on average in the BZ so that $\mathbf{Ch}=0$, θ can be nonzero and may take any real value in general. The value of θ has measurable consequences as it contributes to the magneto-electric coupling in a 3D band insulator.[57] For 3D band insulators with either spin-orbit coupling that are time-reversal symmetric (symmetry class AII) or with chiral symmetry (symmetry class AIII), θ is restricted to integer multiples of π and represents a topological invariant.[19] The 3-bracket (2.88a) shows that for 3D tight-binding Hamiltonians within the symmetry classes AII or AIII, the 3-bracket of the momentum derivatives of projected density operators is dominated by the value of their topological invariant θ, just as the 2-bracket (commutator) of the momentum derivatives of projected density operators is dominated by the value of the Chern number in 2D tight-binding models within the symmetry class A. We will illustrate this statement with the help of a microscopic lattice model belonging to the symmetry class AIII in the Sec. III.

III. NONINTERACTING THREE-BAND TIGHT-BINDING MODEL

The goal of this section is to define a "simple" single-particle Bloch Hamiltonian that supports a dispersionless isolated band with nontrivial topological character, such that the 3-bracket of the momentum derivatives of the projected electronic density operators, Eq. (2.88a), is nonvanishing and the system displays intrinsically 3D physics, i.e., $\mathrm{Ch}^\lambda=0$ for $\lambda=1,2,3$ and $\theta=\pi$. Our model belongs to symmetry class AIII and has three bands, which is the minimum number required to realize the desired θ-term.[57] One of the three bands is necessarily dispersionless as a consequence of chiral symmetry. Therefore, it can be taken as the basis for the construction of fractional topological states in 3D.

A. Definition

We consider spinless electrons hopping between the sites $\boldsymbol{r}^\mathsf{T}\equiv(r_1,r_2,r_3)$ of a 3D cubic lattice Λ and on-site orbitals, whereby each site $\boldsymbol{r}$ can accommodate three orbital degrees of freedom that we label with the Greek index $\alpha=1,2,3$. To accommodate the hybridization between any of the three orbitals, we need to choose a basis for all 3×3 Hermitian matrices. We denote the unit 3×3 matrix by λ_0 which, together with the eight traceless Gell-Mann Hermitian matrices λ_n with $n=1,\cdots,8$, form the desired basis of all 3×3 Hermitian matrices. The second quantized tight-binding Hamiltonian is then defined by

$$\begin{aligned}\widehat{H}:=&\frac{1}{2}\sum_{\boldsymbol{r}\in\Lambda}\sum_{j=1}^{3}\Big[\widehat{c}^\dagger_{\boldsymbol{r}}\left(\mathrm{i}\lambda_{3+j}-\lambda_7\right)\widehat{c}_{\boldsymbol{r}+\boldsymbol{e}_j}+\mathrm{h.c.}\Big]\\&+M\sum_{\boldsymbol{r}\in\Lambda}\widehat{c}^\dagger_{\boldsymbol{r}}\,\lambda_7\,\widehat{c}_{\boldsymbol{r}},\end{aligned} \tag{3.1}$$

where we have introduced the 3-component operator $\widehat{c}^\dagger_{\boldsymbol{r}}\equiv\left(\widehat{c}^\dagger_{\boldsymbol{r};1},\widehat{c}^\dagger_{\boldsymbol{r};2},\widehat{c}^\dagger_{\boldsymbol{r};3}\right)$ with $\widehat{c}^\dagger_{\boldsymbol{r};\alpha}$ creating a spinless fermion at site $\boldsymbol{r}$ in the orbital $\alpha=1,2,3$ and obeying periodic boundary conditions under the translation $\boldsymbol{r}\to\boldsymbol{r}+L\boldsymbol{e}_j$ for any of the three orthonormal unit vectors $\boldsymbol{e}_1$, $\boldsymbol{e}_2$, and $\boldsymbol{e}_3$ that span the cubic lattice Λ. This single-particle Hamiltonian depends on the real-valued parameter M.

Translation invariance allows to diagonalize Hamiltonian (3.1) upon performing a Fourier transformation on the creation and annihilation fermionic operators. If we denote with BZ the Brillouin zone of the 3D cubic lattice and with $\boldsymbol{k}$ any Bloch momentum from the BZ that is

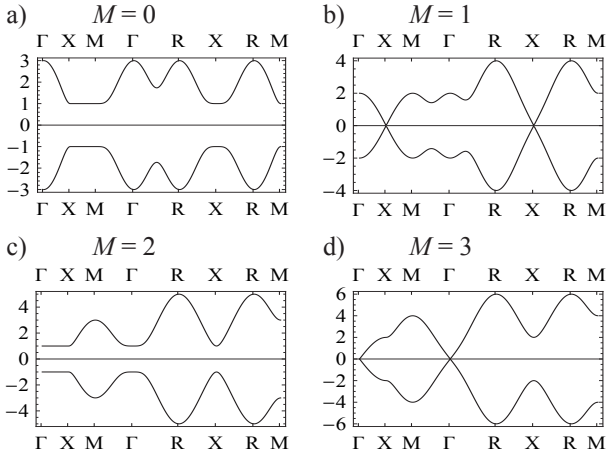

FIG. 2: Energy spectrum of the lattice model defined in Eq. (3.2) for different values of the parameter M. Panels b) and d) show the gap-closing topological transitions. Note the dispersionless band at zero energy in each spectrum. The spectrum is plotted along the straight path connecting the following points in the BZ: $\Gamma = (0,0,0)$, $X = (0,\pi,0)$, $M = (\pi,\pi,0)$, and $R = (\pi,\pi,\pi)$.

compatible with the periodic boundary conditions, then

$$\widehat{H} = \sum_{\boldsymbol{k}\in \mathrm{BZ}} \widehat{c}^{\,\dagger}_{\boldsymbol{k}}\, \mathcal{H}_{\boldsymbol{k}}\, \widehat{c}_{\boldsymbol{k}} \tag{3.2a}$$

with the momentum-resolved single-particle 3×3 matrix

$$\mathcal{H}_{\boldsymbol{k}} = \sum_{j=1}^{4} \lambda_{3+j}\, d_{\boldsymbol{k},j} \tag{3.2b}$$

that depends on the 4-component real-valued row vector

$$\begin{aligned} d^{\mathsf{T}}_{\boldsymbol{k}} &\equiv \left(d_{\boldsymbol{k},1}, d_{\boldsymbol{k},2}, d_{\boldsymbol{k},3}, d_{\boldsymbol{k},4}\right) \\ &:= \left(\sin k_1, \sin k_2, \sin k_3, M - \sum_{i=1}^{3} \cos k_i\right). \end{aligned} \tag{3.2c}$$

With the help of the explicit representation of the eight Gell-Mann matrices from Appendix B, one verifies that

$$\mathcal{C}\, \mathcal{H}_{\boldsymbol{k}}\, \mathcal{C}^{-1} = -\mathcal{H}_{\boldsymbol{k}}, \qquad \forall \boldsymbol{k} \in \mathrm{BZ}, \tag{3.3a}$$

if and only if the 3×3 matrix $\mathcal{C}$ is given by

$$\mathcal{C} := \mathrm{diag}(1,1,-1). \tag{3.3b}$$

The fact that $\mathcal{H}_{\boldsymbol{k}}$ anticommutes with $\mathcal{C}$ implies that any pair of eigenstates $u^{(+)}_{\boldsymbol{k}}$ and $u^{(-)}_{\boldsymbol{k}}$ of $\mathcal{H}_{\boldsymbol{k}}$ with nonvanishing eigenvalues is associated with the opposite single-particle eigenenergies $\varepsilon^{(+)}_{\boldsymbol{k}} = -\varepsilon^{(-)}_{\boldsymbol{k}}$, respectively. Since $\mathcal{H}_{\boldsymbol{k}}$ is a 3×3 Hermitian matrix for any momentum $\boldsymbol{k}$ from the BZ, it then follows that at least one eigenstate $u^{(0)}_{\boldsymbol{k}}$ must have the vanishing eigenvalue

$$\varepsilon^{(0)}_{\boldsymbol{k}} = 0, \tag{3.4a}$$

irrespective of the Bloch momentum $\boldsymbol{k}$ in the BZ. For any Bloch momentum $\boldsymbol{k}$ in the BZ, the values taken by the nonvanishing eigenvalues

$$\varepsilon^{(+)}_{\boldsymbol{k}} = -\varepsilon^{(-)}_{\boldsymbol{k}} = |d_{\boldsymbol{k}}| \tag{3.4b}$$

follow immediately from the fact that the four Gell-Mann matrices λ_4, λ_5, λ_6, and λ_7, anticommute pairwise while any one of these 4 Gell-Mann matrices squares to either $\mathrm{diag}(1,0,1)$ or $\mathrm{diag}(0,1,1)$. The minimum value reached by the magnitude $|d_{\boldsymbol{k}}|$ over the BZ thus determines the energy gap between the dispersionless band of zero modes and the pair of bands related by the chiral transformation $\mathcal{C}$. This energy gap depends parametrically on M and is nonvanishing if and only if $|M| \neq 1, 3$. In turn, the corresponding Bloch states are derived as follows. One observes that the 2-component complex-valued row vector

$$q^{\dagger}_{\boldsymbol{k}} := |d_{\boldsymbol{k}}|^{-1} \left(d_{\boldsymbol{k};1} + \mathrm{i} d_{\boldsymbol{k};2}, d_{\boldsymbol{k};3} + \mathrm{i} d_{\boldsymbol{k};4}\right) \tag{3.5a}$$

of unit length ($q^{\dagger}_{\boldsymbol{k}}\, q_{\boldsymbol{k}} = 1$) enters $\mathcal{H}_{\boldsymbol{k}}$ according to

$$\begin{aligned} \mathcal{H}_{\boldsymbol{k}} &= |d_{\boldsymbol{k}}| \begin{pmatrix} 0 & 0 & q_{\boldsymbol{k},1} \\ 0 & 0 & q_{\boldsymbol{k},2} \\ q^{*}_{\boldsymbol{k},1} & q^{*}_{\boldsymbol{k},2} & 0 \end{pmatrix} \\ &\equiv |d_{\boldsymbol{k}}| \begin{pmatrix} 0_{2\times 2} & q_{\boldsymbol{k}} \\ q^{\dagger}_{\boldsymbol{k}} & 0 \end{pmatrix}. \end{aligned} \tag{3.5b}$$

One then verifies that

$$u^{(\pm)}_{\boldsymbol{k}} = \frac{1}{\sqrt{2}} \begin{pmatrix} +q_{\boldsymbol{k},1} \\ +q_{\boldsymbol{k},2} \\ \pm 1 \end{pmatrix}, \qquad u^{(0)}_{\boldsymbol{k}} = \begin{pmatrix} +q^{*}_{\boldsymbol{k};2} \\ -q^{*}_{\boldsymbol{k};1} \\ 0 \end{pmatrix} \tag{3.5c}$$

are orthonormal Bloch states of $\mathcal{H}_{\boldsymbol{k}}$ for any Bloch momentum $\boldsymbol{k}$ from the BZ. For any value of the parameter M entering the single-particle Hamiltonian $\widehat{H}$, Eqs. (3.5c) and (3.4) define globally over the entire BZ the desired Bloch states with their dispersions. For generic values of M, i.e., whenever $|d_{\boldsymbol{k}}|$ is nonvanishing over the entire BZ, there are two dispersive bands whose Bloch states $u^{(+)}_{\boldsymbol{k}} = \mathcal{C}\, u^{(-)}_{\boldsymbol{k}}$ are related by the chiral transformation and one dispersionless band $u^{(0)}_{\boldsymbol{k}} = \mathcal{C}\, u^{(0)}_{\boldsymbol{k}}$ of zero modes.

Hamiltonian (3.2) breaks time-reversal symmetry, for the first three components of $d_{\boldsymbol{k}}$ are odd while the fourth component is even under $\boldsymbol{k} \to -\boldsymbol{k}$ for any value of M. This leaves no room for a particle-hole symmetry by which Hamiltonian (3.2) would anticommute with an antiunitary operator. Adding to Hamiltonian (3.2) any linear combination of the remaining Gell-Mann matrices λ_1, λ_2, λ_3, λ_8, and the unit 3×3 matrix λ_0 breaks the chiral symmetry. Such perturbations change the symmetry class of Hamiltonian (3.2) from AIII to A. Although a chemical potential (a nonvanishing constant term proportional to the unit matrix λ_0) does break the chiral symmetry, it does so by moving rigidly the entire energy spectrum up or down in energy while leaving the

Bloch states unchanged. The topological attributes of the three Bloch bands are thus untouched by the addition of a chemical potential.

B. Topological invariants

We shall take the thermodynamic limit $L \to \infty$ with L the linear extend over which periodic boundary conditions are imposed. In this limit sums over momenta in the BZ are replaced by integrals over the BZ while the index $\boldsymbol{k}$ becomes the argument of functions. From now on, we shall identify the BZ with T^3. We can then distinguish two related topological invariants associated to the family of single particle 3×3 matrices $\mathcal{H}(\boldsymbol{k})$ labeled by the momentum $\boldsymbol{k}$ from a BZ with the topology of the 3-torus T^3 owing to the periodic boundary conditions.

The first topological attribute characterizes the bundle of Hamiltonians $\mathcal{H}(\boldsymbol{k})$ over the BZ T^3. For any momentum $\boldsymbol{k} \in T^3$, there is a one-to-one correspondence between the 3×3 Hermitian matrices $\mathcal{H}(\boldsymbol{k})$ and the vector $d(\boldsymbol{k}) \in \mathbb{R}^4$. For any momentum $\boldsymbol{k} \in T^3$, the magnitude $|d(\boldsymbol{k})|$ measures the momentum-resolved energy separation between the zero mode $u^{(0)}(\boldsymbol{k})$ and the lower and upper modes $u^{(-)}(\boldsymbol{k})$ and $u^{(+)}(\boldsymbol{k})$, respectively. The eigenstates $u^{(0)}(\boldsymbol{k})$, $u^{(-)}(\boldsymbol{k})$, and $u^{(+)}(\boldsymbol{k})$ are independent of the magnitude of $|d(\boldsymbol{k})|$, i.e., they only depend on the coordinate defined by the unit 3-vector $d(\boldsymbol{k})/|d(\boldsymbol{k})|$ on the 3-sphere S^3 . It follows that the topological attributes of the three Bloch bands of Hamiltonian (3.2) are determined by the homotopy group $\mathbb{Z}$ of the map defined by

$$\boldsymbol{k} \in T^3 \to d(\boldsymbol{k})/|d(\boldsymbol{k})| \in S^3 \tag{3.6}$$

between the BZ T^3 and the 3-sphere S^3. For each parameter $M \neq \pm 1, \pm 3$ entering in Hamiltonian (3.2), the integer value taken by the topological invariant

$$\nu(M) := \frac{1}{12\pi^2} \int_{T^3} \mathrm{d}^3\boldsymbol{k}\, \epsilon^{ijkl}\, \epsilon^{\mu\nu\lambda}\, \frac{1}{|d|^4} d_i\, \partial_\mu d_j\, \partial_\nu d_k\, \partial_\lambda d_l\,, \tag{3.7a}$$

determines which homotopy class the map (3.6) belongs to. Here, we are using the short-hand notation $\partial_\mu d_j \equiv \partial d_j/dk^\mu$, with μ, ν, λ labeling the three coordinates of the momentum $\boldsymbol{k}$ and i, j, k, l labeling the four components of the vector field d, and the convention for summation over repeated indices. Explicit computation of ν as a function of M delivers

$$\nu(M) = \begin{cases} +2, & |M| < 1, \\ -1, & 1 < |M| < 3, \\ 0, & 3 < |M|. \end{cases} \tag{3.7b}$$

Whenever $|M| = 1, 3$, the gap over the BZ closes at the discrete points (the lattice spacing is unity)

$$\boldsymbol{k}^{\mathsf{T}}_{lmn} := \pi\,(l, m, n), \qquad l, m, n = 0, 1. \tag{3.8}$$

These eight momenta change by a reciprocal wave vector under the operation of time reversal, under which $\boldsymbol{k} \to -\boldsymbol{k}$. In this sense, they are time-reversal invariant. The touching of the upper and lower dispersions at the momenta (3.8) occurs at zero energy and delivers a Dirac dispersion in their close vicinity when $|M| = 1, 3$. Hence, we call the momenta (3.8) Dirac points when $|M| = 1, 3$. For small deviations away from $|M| = 1, 3$, a spectral gap opens up at the momenta (3.8) that can be associated with a Dirac mass. Remarkably, the number of Dirac points that change the sign of their mass across a transition tuned by changing M through any one of the values $|M| = 1, 3$ is equal to the change in the topological invariants (3.7). To see this, observe that the momentum resolved Dirac masses are given by

$$\begin{aligned} &d_{\boldsymbol{k}_{000};4} = M - 3, \\ &d_{\boldsymbol{k}_{001};4} = d_{\boldsymbol{k}_{010};4} = d_{\boldsymbol{k}_{100};4} = M - 1, \\ &d_{\boldsymbol{k}_{110};4} = d_{\boldsymbol{k}_{101};4} = d_{\boldsymbol{k}_{011};4} = M + 1, \\ &d_{\boldsymbol{k}_{111};4} = M + 3. \end{aligned} \tag{3.9}$$

With the help of these 8 integers, we define the integer

$$\nu_{\mathrm{D}}(M) := \frac{1}{2} \sum_{m,n,l=0,1} (-1)^{m+n+l}\, \mathrm{sign}\, d_{\boldsymbol{k}_{mnl};4}. \tag{3.10}$$

The factor $(-1)^{m+n+l}$ assures that the mass sign is taken relative to the chirality of the kinetic piece of the Dirac operator. One verifies that (see also Appendix D)

$$\nu_{\mathrm{D}}(M) = \nu(M) \tag{3.11}$$

for any $|M| \neq 1, 3$.

The second topological attribute characterizes the bundle of Bloch states $u^{(\tilde{a})}(\boldsymbol{k})$ over the BZ T^3 for any of the three bands $\tilde{a} = -, 0, +$. Whenever $|M| \neq 1, 3$, it is nothing but the triplet of Berry phases[75]

$$\theta^{(\tilde{a})}(M) := \frac{1}{4\pi} \int_{T^3} \mathrm{d}^3\boldsymbol{k}\, \epsilon^{\mu\nu\lambda}\, A^{(\tilde{a})}_\mu\, \partial_\nu\, A^{(\tilde{a})}_\lambda, \tag{3.12a}$$

where we have introduced the Abelian Berry connection

$$A^{(\tilde{a})}_\mu(\boldsymbol{k}) := \left(u^{(\tilde{a})\dagger} \frac{\partial}{\partial k^\mu} u^{(\tilde{a})} \right)(\boldsymbol{k}) \tag{3.12b}$$

for any of the three bands $\tilde{a} = -, 0, +$. With the help of Eq. (3.5c), one deduces that

$$\theta^{(0)}(M) = \frac{1}{4\pi} \int_{T^3} \mathrm{d}^3\boldsymbol{k}\, \epsilon^{\mu\nu\lambda}\, \left(q^\dagger\, \partial_\mu q\, \partial_\nu q^\dagger\, \partial_\lambda q \right)(\boldsymbol{k}) \tag{3.13a}$$

and

$$\theta^{(-)}(M) = \theta^{(+)}(M) = \frac{1}{4}\theta^{(0)}(M) \tag{3.13b}$$

when $|M| \neq 1, 3$. Explicit evaluations of the Berry phase of any of the three bands then yields

$$\theta^{(-)}(M) = \theta^{(+)}(M) = \frac{1}{4}\theta^{(0)}(M) = \frac{\pi}{4}\nu(M) \qquad (3.14)$$

when $|M| \neq 1, 3$ (see Appendix C).

With this computation of the topological invariant θ, we have also established that the projected electronic density in any of the bands of 3-orbital model obeys the noncommutative 3-bracket defined in Eq. (2.88a) that is dominated by the value of θ. Upon partial filling, the flat middle band thus provides a manifold of many-body non-interacting ground states with macroscopic ground state degeneracy, similar to the case of a partially filled Landau level. Henceforth, one may expect interesting many-body ground states to appear once electron-electron interactions are added to the model. In that regard, we observe that any many-body Hamiltonian that includes an interaction build out of density operators projected to the middle band is invariant under the chiral transformation (3.3a), since the projected density operators themselves are invariant under the chiral transformation (3.3a).

C. Surface states

We shall here provide an interpretation of the topological invariant (3.10) as a manifestation of the surface states associated with a spatially dependent mass parameter M in the Hamiltonian (3.2). This observation applies when considering the surface states that connect bands separated by a bulk gap. Such surface states, connecting the upper and lower band, appear only when the periodic boundary conditions are replaced by open boundary conditions that implement a slab geometry with the surface normal parallel to the r_3 direction.

In order to study the surface modes, we consider the low energy description of the Hamiltonian (3.2) by linearizing it around each of the 8 nodal points in the Brillouin zone $\boldsymbol{k}^{\mathsf{T}}_{lmn} = \pi(l, m, n)$, with $l, m, n = 0, 1$. The Hamiltonian (3.2) in the linearized approximation factorizes according to

$$\mathcal{H} = \bigotimes_{l,m,n=0,1} \mathcal{H}_{lmn}. \qquad (3.15)$$

For example, the expansion $\mathcal{H}$ around $\boldsymbol{k}^{\mathsf{T}}_{000}$ produces

$$\mathcal{H}_{000} = \begin{pmatrix} 0 & 0 & \hat{k}_- \\ 0 & 0 & \hat{k}_3 - \mathrm{i}\, M_{000} \\ \hat{k}_+ & \hat{k}_3 + \mathrm{i}\, M_{000} & 0 \end{pmatrix}, \qquad (3.16)$$

where $\hat{k}_\pm \equiv \hat{k}_1 \pm \mathrm{i}\hat{k}_2$, $\hat{k}_j \equiv -\mathrm{i}\partial_{r_j}$, for $j = 1, 2, 3$ and $M_{000} = M - 3$. For a uniform mass M_{000}, the spectrum breaks into three low energy bands with eigenvalues 0 and $\pm\sqrt{\boldsymbol{k}^2 + |M_{000}|^2}$.

We now regard M_{000} as a domain wall configuration along the r_3-direction, which we choose to parametrize as

$$M_{000}(r_3) = \overline{M}_{000}\left[\Theta(r_3) - \Theta(-r_3)\right], \qquad (3.17)$$

where Θ is the Heaviside function. The choice of a sharp domain wall in (3.17) facilitates the analytic treatment of the eigenmode equations and does not affect the generality of the following discussion. Due to the translational invariance on the $\boldsymbol{e}_1$-$\boldsymbol{e}_2$ plane, we seek solutions of

$$\mathcal{H}_{000}\,\psi_{000,\boldsymbol{\kappa}} = \varepsilon_{\boldsymbol{\kappa}}\,\psi_{000,\boldsymbol{\kappa}}, \qquad (3.18)$$

with $\psi_{000,\boldsymbol{\kappa}}(\boldsymbol{\rho}, r_3) = e^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{\rho}}\,\phi_{000,\boldsymbol{k}}(r_3)$, whereby $\boldsymbol{\rho} = (r_1, r_2)$ and $\boldsymbol{\kappa} = (k_1, k_2)$ are, respectively, the coordinates and momenta projected on the $\boldsymbol{e}_1$-$\boldsymbol{e}_2$ plane. The components of the spinor wavefunction

$$\phi_{000,\boldsymbol{\kappa}}(r_3) = \big(f_{\boldsymbol{\kappa}}(r_3), g_{\boldsymbol{\kappa}}(r_3), h_{\boldsymbol{\kappa}}(r_3)\big)^{\mathsf{T}} \qquad (3.19)$$

satisfy

$$f_{\boldsymbol{\kappa}}(r_3) = \frac{k_-}{\varepsilon_{\boldsymbol{\kappa}}} h_{\boldsymbol{\kappa}}(r_3), \qquad (3.20a)$$

$$g_{\boldsymbol{\kappa}}(r_3) = \frac{1}{\varepsilon_{\boldsymbol{\kappa}}}\left[-\mathrm{i}\partial_{r_3} - \mathrm{i}M_{000}(r_3)\right] h_{\boldsymbol{\kappa}}(r_3), \qquad (3.20b)$$

and

$$\begin{aligned}\left[-\partial^2_{r_3} + M^2_{000}(r_3) - 2\overline{M}_{000}\delta(r_3)\right] h_{\boldsymbol{\kappa}}(r_3) \\ = (\varepsilon^2_{\boldsymbol{\kappa}} - \boldsymbol{\kappa}^2) h_{\boldsymbol{\kappa}}(r_3).\end{aligned} \qquad (3.20c)$$

At $r_3 \neq 0$, the solution of Eq. (3.20c) yields

$$h_{\boldsymbol{\kappa}}(r_3) = h_0\, e^{-|r_3|/\lambda}, \qquad (3.21)$$

where h_0 is a normalization constant and $\lambda^{-1} := \sqrt{\overline{M}^2_{000} + \boldsymbol{\kappa}^2 - \varepsilon^2_{\boldsymbol{\kappa}}} > 0$, while the delta function discontinuity at $r_3 = 0$ imposes the condition $\lambda^{-1} = \overline{M}_{000}$. Therefore, the domain wall configuration (3.17) bounds surface states with dispersion

$$\varepsilon_{\pm,\boldsymbol{\kappa}} = \pm|\boldsymbol{\kappa}| \qquad (3.22)$$

provided $\overline{M}_{000} > 0$. Evaluating the solution (3.21) in (3.20a) and (3.20b) yields the spinor wavefunction, which, up to a normalization constant $\mathcal{N}$, reads

$$\psi_{000,\pm,\boldsymbol{\kappa}}(\boldsymbol{\rho}, r_3) = \mathcal{N}\,\varphi_{000,\pm,\boldsymbol{\kappa}}\, e^{\mathrm{i}\boldsymbol{\kappa}\cdot\boldsymbol{\rho}}\, e^{-\overline{M}_{000} r_3}, \qquad (3.23a)$$

$$\varphi_{000,\pm,\boldsymbol{\kappa}} = 2^{-1/2}\left(\pm e^{-\mathrm{i}\alpha_{\boldsymbol{\kappa}}}, 0, 1\right)^{\mathsf{T}}, \quad \frac{k_\pm}{|\boldsymbol{\kappa}|} \equiv e^{\pm\mathrm{i}\alpha_{\boldsymbol{\kappa}}}. \qquad (3.23b)$$

The discussion of the boundary states of the low energy Hamiltonians with $n = 0$, $\mathcal{H}_{lm0}$, is very similar to that of

$\mathcal{H}_{000}$. In this case, the existence of gapless surface states with dispersion as in Eq. (3.22) for sharp domain wall configurations

$$M_{lm0}(z) = \overline{M}_{lm0}\left[\theta(r_3) - \theta(-r_3)\right] \tag{3.24}$$

requires $\overline{M}_{lm0} > 0$. The explicit form of the eigenspinors (omitting the r_3 dependent part) is

$$\begin{aligned}
\varphi_{00n,\pm,\boldsymbol{\kappa}} &= 2^{-1/2}\left(\pm e^{-\mathrm{i}\alpha_{\boldsymbol{k}}}, 0, 1\right)^{\mathsf{T}}, \\
\varphi_{10n,\pm,\boldsymbol{\kappa}} &= 2^{-1/2}\left(\mp e^{+\mathrm{i}\alpha_{\boldsymbol{k}}}, 0, 1\right)^{\mathsf{T}}, \\
\varphi_{11n,\pm,\boldsymbol{\kappa}} &= 2^{-1/2}\left(\mp e^{-\mathrm{i}\alpha_{\boldsymbol{k}}}, 0, 1\right)^{\mathsf{T}}, \\
\varphi_{01n,\pm,\boldsymbol{\kappa}} &= 2^{-1/2}\left(\pm e^{+\mathrm{i}\alpha_{\boldsymbol{k}}}, 0, 1\right)^{\mathsf{T}},
\end{aligned} \tag{3.25}$$

where $n = 0$. For the boundary states of the low energy Hamiltonians with $n = 1$, $\mathcal{H}_{lm1}$, the extra minus sign coming from the Taylor expansion around $k_3 = \pi$ implies that the gapless surface states exist for domain wall configurations

$$M_{lm1}(r_3) = \overline{M}_{lm1}\left[\theta(r_3) - \theta(-r_3)\right], \tag{3.26}$$

provided $\overline{M}_{lm1} < 0$. The eigenspinors in this case are given by Eq. (3.25) with $n = 1$.

In order to account for all the possible surface modes in a finite size configuration, we now take, for the sake of concreteness, our system to be a slab, infinite in the $\boldsymbol{e}_1$-$\boldsymbol{e}_2$ plane and confined in the r_3-direction by $r_3^{\mathrm{top}} \leq r_3 \leq r_3^{\mathrm{bottom}}$, with $r_3^{\mathrm{top}} - r_3^{\mathrm{bottom}}$ assumed to be much larger than any other length scale so as to regard the two surfaces as completely decoupled from each other. Moreover, let us adopt the convention that the vacuum is characterized by a positive value of the gap parameter ($M_{\mathrm{vac}} > 0$), which then changes to negative values for $r_3^{\mathrm{top}} < r_3 < r_3^{\mathrm{bottom}}$. For this particular configuration, the discussion above implies the presence of gapless surface states associated with $\mathcal{H}_{lm0}$ ($\mathcal{H}_{lm1}$) at the surface $r_3 = r_3^{\mathrm{top}}$ ($r_3 = r_3^{\mathrm{bottom}}$) for $\overline{M}_{lm0} < 0$ ($\overline{M}_{lm1} < 0$).

In order to make a connection with the topological invariant (3.10) we now compute the winding number of the eigenspinors as

$$\nu_{lm0} = +\frac{1}{\pi\,\mathrm{i}} \oint \mathrm{d}\boldsymbol{\kappa} \cdot \left(\varphi^{\dagger}_{lm0,\pm,\boldsymbol{\kappa}} \boldsymbol{\nabla}_{\boldsymbol{\kappa}} \varphi_{lm0,\pm,\boldsymbol{\kappa}}\right), \tag{3.27a}$$

$$\nu_{lm1} = -\frac{1}{\pi\,\mathrm{i}} \oint \mathrm{d}\boldsymbol{\kappa} \cdot \left(\varphi^{\dagger}_{lm1,\pm,\boldsymbol{\kappa}} \boldsymbol{\nabla}_{\boldsymbol{\kappa}} \varphi_{lm1,\pm,\boldsymbol{\kappa}})\right), \tag{3.27b}$$

where the explicit overall sign difference between (3.27a) and (3.27b) reflects the opposite orientation of the outward normal vectors $+\boldsymbol{e}_3$ and $-\boldsymbol{e}_3$ at the surfaces $r_3 = r_3^{\mathrm{top}}$ and $r_3 = r_3^{\mathrm{bottom}}$, respectively. Direct computation using Eq. (3.25) gives

$$\nu_{000} = \nu_{110} = \nu_{101} = \nu_{011} = -1, \tag{3.28a}$$

$$\nu_{100} = \nu_{010} = \nu_{001} = \nu_{111} = +1. \tag{3.28b}$$

The total winding number of the surface states is encoded in the quantity

$$\tilde{\nu} \equiv \sum_{\overline{M}_{lmn}<0} \nu_{lmn}, \tag{3.29}$$

which acquires the following values:

$$\tilde{\nu} = \begin{cases} +2, & |M| < 1, \\ -1, & 1 < |M| < 3, \\ 0, & 3 < |M|. \end{cases} \tag{3.30}$$

Comparison between Eq. (3.30) and Eq. (3.7b) thus establishes a direct relationship between the topological index (3.10) and the total winding number of the surface states $\tilde{\nu}$. Similar analysis of the finite size system spectrum for domain wall configurations of the gap parameter along either the x or the y directions reveals the nonexistence of surface states.

IV. INTERACTIONS WITHIN THE SINGLE-MODE APPROXIMATION

We begin by reviewing the single-mode approximation (SMA) to the FQHE from Ref. 33.

In the IQHE, the external magnetic field organizes the single-particle spectrum into degenerate Landau levels, whereby two consecutive Landau levels are separated by the energy gap $\hbar\omega_c$. The cyclotron frequency $\omega_c = \hbar/(m_{\mathrm{e}}\ell_B^2)$ is proportional to the magnitude B of the uniform magnetic field.

We consider the limit of very strong magnetic fields relative to the characteristic energy scale V of the electron-electron interactions, i.e., $\hbar\omega_c \gg V$. Moreover, we consider a filling fraction $\nu \equiv \Phi/\Phi_0 < 1$ (Φ the magnetic flux and Φ_0 the flux quantum) such that the exact many-body ground state $|\Psi_0\rangle$ does not break spontaneously any symmetry. The translation invariant interacting Hamiltonian $\widehat{H}$ describing a nonvanishing density of spinless fermions moving in a plane perpendicular to an external magnetic field of uniform magnitude B and interacting pairwise with a (screened) Coulomb interaction is then well approximated, as far as low energy properties go, by its projection $\widehat{H}_{\mathrm{LLL}}$ onto the vector space spanned by the lowest Landau single-particle levels.

Upon imposing periodic boundary conditions in an area of linear size L, $\widehat{H}_{\mathrm{LLL}}$ is given by

$$\widehat{H}_{\mathrm{LLL}} = \sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\, \delta\widehat{\rho}_{-\boldsymbol{q}}\, \delta\widehat{\rho}_{+\boldsymbol{q}}, \tag{4.1a}$$

where

$$v_{\boldsymbol{q}} = v^{*}_{\boldsymbol{q}} = v_{-\boldsymbol{q}} \tag{4.1b}$$

is the Fourier transform of the screened Coulomb interaction, while

$$\delta\widehat{\rho}_{\boldsymbol{q}} := \widehat{\rho}_{\boldsymbol{q}} - \left\langle\, \Psi_0 \,\middle|\, \widehat{\rho}_{\boldsymbol{q}} \,\middle|\, \Psi_0 \right\rangle \tag{4.1c}$$

is the Fourier component of the fermion density operator after projection into the LLL measured relative to its expectation value in the exact many-body ground state $|\Psi_0\rangle$.

Inspired by the early work of Feynman and Bijl in their study of excitations in ^{4}He,[34] GMP in Ref. 33 consider the variational state

$$|\phi_{\boldsymbol{k}}\rangle := \delta\widehat{\rho}_{\boldsymbol{k}}\,|\Psi_0\rangle, \tag{4.2}$$

whose energy expectation value $\Delta_{\boldsymbol{k}}$, measured relative to the exact ground state energy E_0, sets a variational upper bound on the low excitation spectrum of the LLL-projected Hamiltonian (4.1).

Assuming the inversion symmetry

$$\Delta_{+\boldsymbol{k}} = \Delta_{-\boldsymbol{k}}, \tag{4.3a}$$

a direct calculation using Eqs. (4.1) and (4.2) leads to

$$\Delta_{\boldsymbol{k}} = \frac{f_{\boldsymbol{k}}}{s_{\boldsymbol{k}}}, \tag{4.3b}$$

where

$$f_{\boldsymbol{k}} = \frac{1}{2}\,\left\langle \Psi_0 \,\middle|\, \left[\delta\widehat{\rho}_{-\boldsymbol{k}}, \left[\widehat{H}_{\mathrm{LLL}}, \delta\widehat{\rho}_{+\boldsymbol{k}}\right]\right] \middle|\, \Psi_0 \right\rangle \tag{4.3c}$$

and

$$s_{\boldsymbol{k}} = \left\langle \Psi_0 \left| \delta\widehat{\rho}_{-\boldsymbol{k}}\,\delta\widehat{\rho}_{+\boldsymbol{k}} \right| \Psi_0 \right\rangle. \tag{4.3d}$$

One recognizes on the right-hand side of Eq. (4.3d) the static structure factor. The insight of GMP in Ref. 33 was to realize that the density operators projected onto the lowest Landau level close the exact algebra

$$\left[\widehat{\rho}_{\boldsymbol{q}}, \widehat{\rho}_{\boldsymbol{k}}\right] = 2\mathrm{i}\,\sin\left(\frac{1}{2}\,(\boldsymbol{q}\times\boldsymbol{k})\cdot\boldsymbol{e}_3\,\ell_B^2\right)\widehat{\rho}_{\boldsymbol{q}+\boldsymbol{k}} \tag{4.4}$$

(ℓ_B is the magnetic length). In turn, the algebra (4.4) implies that

$$f_{\boldsymbol{k}} \sim |\boldsymbol{k}|^4 \tag{4.5}$$

in the small $|\boldsymbol{k}|$ limit. Hence, in the FQHE, a necessary (but not sufficient) condition for the existence of a finite gap in the thermodynamic limit is to have

$$s_{\boldsymbol{k}} \sim |\boldsymbol{k}|^4 \tag{4.6}$$

also hold in the small $|\boldsymbol{k}|$ limit. In fact, Eq. (4.6) was shown in Ref. 33 to be satisfied when $|\Psi_0\rangle$ is chosen to be any Laughlin state with filling fraction $\nu = 1/m$, where m is an odd integer.

In the spirit of GMP, our starting point is a single-particle Hamiltonian defined on a d-dimensional Bravais lattice and sharing its point group symmetry. We also assume that there exists at least one band that is independent of the lattice momentum, i.e., a flat band, and, furthermore, that is separated from the other bands by a single-particle gap Δ. We constructed a 3D example thereof in Sec. III. We then imagine switching on adiabatically a pairwise interaction that preserves the Bravais lattice point-group symmetry, say a (screened) Coulomb interaction. We shall denote with V the corresponding characteristic interaction energy scale. In the regime for which $\Delta \gg V$, Hamiltonian (4.1) can be reinterpreted as the interacting Hamiltonian projected onto this flat band, provided we identify $v_{\boldsymbol{q}}$ with the Fourier transform at the lattice momentum $\boldsymbol{q}$ of the pairwise fermion interaction, $\delta\widehat{\rho}_{\boldsymbol{q}}$ with the Fourier transform at lattice momentum $\boldsymbol{q}$ of the projected operator describing density fluctuation measured relative to the fermion density with lattice momentum $\boldsymbol{q}$ of the exact many-body ground state $|\Psi_0\rangle$, whereby we assume that $|\Psi_0\rangle$ does not break spontaneously any point-group symmetry of the lattice.

The projected density operator on a flat band reads

$$\begin{aligned}\widehat{\rho}_{\boldsymbol{k}} &= \sum_{\boldsymbol{p}} u_{\boldsymbol{p}}^\dagger \cdot u_{\boldsymbol{p}+\boldsymbol{k}}\,\widehat{\chi}_{\boldsymbol{p}}^\dagger\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{k}} \\ &\equiv \sum_{\boldsymbol{p}} M_{\boldsymbol{p},\boldsymbol{k}}\,\widehat{\chi}_{\boldsymbol{p}}^\dagger\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{k}},\end{aligned} \tag{4.7}$$

where $u_{\boldsymbol{k}} \in \mathbb{C}^N$ is vector-valued (its components range over the number N of orbitals per site of the Bravais lattice), while $\widehat{\chi}_{\boldsymbol{k}}$ and $\widehat{\chi}_{\boldsymbol{k}}^\dagger$ are the annihilation and creation operators, respectively, of single-particle fermionic eigenstates on the isolated flat band with lattice momentum $\boldsymbol{k}$. Hence, they satisfy the canonical fermionic anticommutation relations

$$\left\{\widehat{\chi}_{\boldsymbol{k}}, \widehat{\chi}_{\boldsymbol{k}'}\right\} = \left\{\widehat{\chi}_{\boldsymbol{k}}^\dagger, \widehat{\chi}_{\boldsymbol{k}'}^\dagger\right\} = 0, \quad \left\{\widehat{\chi}_{\boldsymbol{k}}, \widehat{\chi}_{\boldsymbol{k}'}^\dagger\right\} = \delta_{\boldsymbol{k},\boldsymbol{k}'} \tag{4.8}$$

for any pair $\boldsymbol{k}$ and $\boldsymbol{k}'$ of lattice momenta. In carrying out the program laid out in Eq. (4.3) for a general lattice Hamiltonian with a flat band, one notices two immediate obstacles.

The first one arises from the fact that the commutator of two (projected) density operators does not satisfy the algebra (4.4) found by GMP for the FQHE in a uniform magnetic field. However, it was noticed in Ref. 38 that, in the limit of small lattice momenta $\boldsymbol{k}$ and $\boldsymbol{k}'$, the commutation relation between two projected density operators reads

$$\begin{aligned}\left[\,\widehat{\rho}(\boldsymbol{k}), \widehat{\rho}(\boldsymbol{k}')\,\right] = \int_{\boldsymbol{p}} &\Big[\mathrm{i}\,(\boldsymbol{k}\wedge\boldsymbol{k}')\cdot\boldsymbol{\mathcal{B}}(\boldsymbol{p}) + \cdots\Big] \\ &\times \widehat{\chi}^\dagger(\boldsymbol{p})\,\widehat{\chi}(\boldsymbol{p}+\boldsymbol{k}+\boldsymbol{k}')\end{aligned} \tag{4.9a}$$

in the thermodynamic limit $L\to\infty$, whereby the shorthand notation

$$\int_{\boldsymbol{p}} \equiv \int \frac{\mathrm{d}^d\boldsymbol{p}}{(2\pi/L)^d} \tag{4.9b}$$

is used,

$$\boldsymbol{\mathcal{B}}(\boldsymbol{p}) := -\mathrm{i}\,(\boldsymbol{\nabla}\wedge\boldsymbol{A})\,(\boldsymbol{p}) \tag{4.9c}$$

is the (real-valued) Berry field strength of the flat band, and

$$\boldsymbol{A}(\boldsymbol{p}) := \left(u^\dagger \cdot \boldsymbol{\nabla}\, u\right)(\boldsymbol{p}) \tag{4.9d}$$

is the (imaginary-valued) Berry connection of the flat band, while $\cdots$ in Eq. (4.9a) accounts for higher order terms in powers of $\boldsymbol{k}$ and $\boldsymbol{k}'$. Consequently, it was proposed in Ref. 38 that the numerical observation of the FQHE without an external magnetic field in 2D Chern insulators in Refs. 50–53 can be understood on the account that, because in a 2D Chern band insulator the integral of the Berry curvature on the Brillouin zone equals the (nonzero) Chern number, replacing $\boldsymbol{\mathcal{B}}(\boldsymbol{p})$ in Eq. (4.9) by its *average*, implies the GMP algebra (4.4) in the long-wavelength limit. However, we would like to stress that, contrary to the 2D Chern band insulators for which one can associate the notion of an average Berry curvature due to the nonzero Chern number, for the 3D lattice models studied in Secs. II and III, the integral of the Berry curvature vanishes so that replacing $\boldsymbol{\mathcal{B}}(\boldsymbol{p})$ by its average is meaningless. Even for 2D Chern band insulators, the Berry curvature is generically nonuniform; a fact that should be reflected in the exact many-body wavefunction.

The second obstacle to applying the SMA to an interacting lattice model is the fact that no good candidate wavefunction is presently known with which one can compute the static structure factor $s_{\boldsymbol{k}}$ and compare its small $\boldsymbol{k}$ dependence with that of $f_{\boldsymbol{k}}$, as was done by GMP in Ref. 33. Nevertheless, information about the behavior of $f_{\boldsymbol{k}}$ for small $\boldsymbol{k}$ and the requirement of a finite gap in the thermodynamic limit, i.e., $\Delta_{\boldsymbol{k}} \to \Delta_0 \neq 0$ for $\boldsymbol{k} \to 0$, puts a constraint on the static structure factor for small $\boldsymbol{k}$ and, correspondingly, on the correlations of the exact many-body wavefunction.

In Appendix E we discuss in detail the evaluation of the function $f_{\boldsymbol{k}}$ defined in Eq. (4.3c) to lowest order in $\boldsymbol{k}$. Our main result is that, due to the non-closure of the density algebra for any d-dimensional lattice model, the leading contribution to $f(\boldsymbol{k})$ reads

$$\begin{aligned} f(\boldsymbol{k}) = & \int\limits_{\boldsymbol{q}} \int\limits_{\boldsymbol{p}} \int\limits_{\boldsymbol{p}'} v(\boldsymbol{q}) \Big[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{\mathcal{B}}(\boldsymbol{p})\Big] \Big[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{\mathcal{B}}(\boldsymbol{p}')\Big] \Big\langle \hat{n}(\boldsymbol{p})\,\hat{n}(\boldsymbol{p}')\Big\rangle \\ & + \int\limits_{\boldsymbol{q}} \int\limits_{\boldsymbol{p}} v(\boldsymbol{q})\, \frac{\mathrm{i}}{2}\, (\boldsymbol{k}\wedge\boldsymbol{q})\cdot\left(\partial_\mu \boldsymbol{\mathcal{B}}\right)(\boldsymbol{p}) k^\mu \Big[\Big\langle \delta\widehat{\rho}(-\boldsymbol{q})\, \widehat{\chi}^\dagger(\boldsymbol{p})\, \widehat{\chi}(\boldsymbol{p}+\boldsymbol{q})\Big\rangle - \Big\langle \widehat{\chi}^\dagger(\boldsymbol{p}+\boldsymbol{q})\, \widehat{\chi}(\boldsymbol{p})\, \delta\widehat{\rho}(\boldsymbol{q})\Big\rangle\Big] \end{aligned} \tag{4.10a}$$

where $\int\limits_{\boldsymbol{q}} \equiv \int \mathrm{d}^d\boldsymbol{q}/(2\pi/L)^d$ and the summation convention is implied over the repeated index $\mu = 1, \cdots, d$. In Eq. (4.10a),

$$\hat{n}(\boldsymbol{p}) := \widehat{\chi}^\dagger(\boldsymbol{p})\, \widehat{\chi}(\boldsymbol{p}) \tag{4.10b}$$

while

$$\delta\boldsymbol{\mathcal{B}}(\boldsymbol{p}) := \boldsymbol{\mathcal{B}}(\boldsymbol{p}) - \overline{\boldsymbol{\mathcal{B}}} \tag{4.10c}$$

denotes the deviations of the Berry curvature $\boldsymbol{\mathcal{B}}(\boldsymbol{p})$ away from the uniform background value $\overline{\boldsymbol{\mathcal{B}}}$. This uniform background value is defined in such a way that, when $d = 3$,

$$\begin{aligned} \mathrm{Ch}^\lambda :=& 2\pi \times \frac{1}{2} \int\limits_{T^3} \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3} \mathcal{B}^\lambda(\boldsymbol{p}) \\ \equiv & \frac{2\pi}{L^3} \times \frac{1}{2} \int\limits_{T^3} \frac{\mathrm{d}^3\boldsymbol{p}}{(2\pi)^3} \overline{\mathcal{B}}^\lambda \end{aligned} \tag{4.11}$$

with $\lambda = 1, 2, 3$ is compatible with a generalization of the 2D Chern number to layered (quasi-2D) materials. The result (4.10a) should be contrasted with the calculation in Ref. 33, for which the order $\boldsymbol{k}^2$ term in $f(\boldsymbol{k})$ vanishes identically as a consequence of the algebra (4.4). The formula (4.10a) thus establishes a direct relationship, within the SMA, between the deviations of the Berry field strength away from a uniform configuration and the order $\boldsymbol{k}^2$ contribution to $f(\boldsymbol{k})$

$$f(\boldsymbol{k}) \sim |\boldsymbol{k}|^2 \,. \tag{4.12}$$

Such a relation is relevant either for 2D fractional Chern band insulators for which, despite a nonzero Chern number, $\boldsymbol{\mathcal{B}}(\boldsymbol{p})$ can be nonuniform throughout the Brillouin zone or for the general classes of 3D lattice models studied in Secs. II and III for which the integral of $\boldsymbol{\mathcal{B}}(\boldsymbol{p})$ vanishes. The result (4.10a) also indicates that a prerequisite for the existence of a nonvanishing but finite many-body gap to excitations above the many-body ground state is that the static structure factor $s(\boldsymbol{k})$ has also to vanish as $\boldsymbol{k}^2$ to allow for the possibility of a nonzero ratio $\Delta(\boldsymbol{k}) \equiv f(\boldsymbol{k})/s(\boldsymbol{k})$ and therefore a nonvanishing SMA gap in Eq. (4.3b).

V. SUMMARY

The noncommutativity of coordinates and density operators in a featureless liquid-like electronic state can be

a local probe of its topological character. In this paper, we have studied how this fact, which is well-established for quantum Hall fluids in 2D, carries over to 3D topological states of itinerant electrons. In the limit of long wavelength, we found that both the noncommutative relations obeyed by projected position and density operators are characterized by the topological invariant of a 3D band structure with chiral symmetry. We established a relation between the noncommutative relation of the projected position operators and the classical Nambu bracket of volume-preserving diffeomorphisms of 3D fluids, that might bridge the description of classical ideal fluids and that of topological incompressible states in 3D.

One experimental manifestation of band topology are boundary states. Their existence is, in turn, tied to the topological electromagnetic response of the system. On the basis of our results that relate the expectation values of position operators with band topology, we conclude that the noncommutative geometry is observable via response functions. First, the expectation value of the regularized projected position operator itself is the polarization, that is a zeroth-order response, in the sense that it exists without external perturbing fields. The expectation value of the commutator and the 3-bracket of projected position operators describe linear response via the Hall conductivity and the magneto-electric polarizability, respectively. The latter yields the polarization created by application of a magnetic field and has a contribution from the 3D Chern-Simons invariant, or equivalently the θ-term.[57,59]

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Appendix A: Gauge-invariant regularization of brackets of projected position operators

1. Definition of the single-particle Hilbert space

Define the three lattices

$$\Lambda^{\star}_{\rm BZ} := \left\{ (k^\mu) \in \mathbb{R}^d \,\middle|\, k^\mu = \frac{2\pi}{\mathfrak{a}}\, n^\mu, \quad n^\mu = 1, \cdots, \mathcal{N}^\mu \right\}, \tag{A1a}$$

$$\Lambda_r := \left\{ (r^\mu) \in \mathbb{R}^d \,\middle|\, r^\mu = \mathfrak{a}\, n^\mu, \quad n^\mu = 1, \cdots, \mathcal{N}^\mu \right\}, \tag{A1b}$$

and

$$\Lambda_R := \left\{ (R^\mu) \in \mathbb{R}^d \,\middle|\, R^\mu = \mathfrak{a}\, n^\mu, \quad n^\mu = 1, \cdots, \mathcal{N}^\mu \right\}, \tag{A1c}$$

each of which shares the same cardinality

$$\mathcal{N} := \prod_{\mu=1}^{d} \mathcal{N}^\mu. \tag{A2}$$

The lattices Λ_r and Λ_R share the same unit cell of linear extend $\mathfrak{a}$ but they might be shifted by the vector

$$\boldsymbol{d} := \sum_{\mu=1}^{d} e_\mu\, \boldsymbol{e}^\mu, \qquad 0 \le e_\mu < 1, \qquad \boldsymbol{e}^\mu \cdot \boldsymbol{e}^\nu = \delta^{\mu,\nu}, \qquad \mu, \nu = 1, \cdots, d, \tag{A3}$$

from the unit cell relative to each other.

The single-particle Hilbert space is defined through a basis of orthonormal states. We introduce two such bases. There is the orbital basis

$$\mathbb{1} = |\psi^\alpha_{\boldsymbol{r}}\rangle \langle \psi^\alpha_{\boldsymbol{r}}| = |\psi^\alpha_{\boldsymbol{k}}\rangle \langle \psi^\alpha_{\boldsymbol{k}}|, \quad \langle \psi^\alpha_{\boldsymbol{r}} | \psi^{\alpha'}_{\boldsymbol{r}'}\rangle = \delta^{\alpha,\alpha'}\, \delta_{\boldsymbol{r},\boldsymbol{r}'}, \quad \langle \psi^\alpha_{\boldsymbol{k}} | \psi^{\alpha'}_{\boldsymbol{k}'}\rangle = \delta^{\alpha,\alpha'}\, \delta_{\boldsymbol{k},\boldsymbol{k}'}, \quad \langle \psi^\alpha_{\boldsymbol{r}} | \psi^{\alpha'}_{\boldsymbol{k}}\rangle = \delta^{\alpha,\alpha'}\, \frac{1}{\sqrt{\mathcal{N}}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \tag{A4}$$

with the summation convention implied over repeated indices and for any pairs $\alpha, \alpha' = 1, \cdots, N$ or $\boldsymbol{r}, \boldsymbol{r}' \in \Lambda_r$ or $\boldsymbol{k}, \boldsymbol{k}' \in \Lambda^\star_{\text{BZ}}$.

There is the band basis

$$\mathbb{1} = |W^a_{\boldsymbol{R}}\rangle \langle W^a_{\boldsymbol{R}}| = |\chi^a_{\boldsymbol{k}}\rangle \langle \chi^a_{\boldsymbol{k}}|, \quad \langle W^a_{\boldsymbol{R}}|W^{a'}_{\boldsymbol{R}'}\rangle = \delta^{a,a'}\, \delta_{\boldsymbol{R},\boldsymbol{R}'}, \quad \langle \chi^a_{\boldsymbol{k}}|\chi^{a'}_{\boldsymbol{k}'}\rangle = \delta^{a,a'}\, \delta_{\boldsymbol{k},\boldsymbol{k}'}, \quad \langle W^a_{\boldsymbol{R}}|\chi^{a'}_{\boldsymbol{k}}\rangle = \delta^{a,a'}\, \frac{1}{\sqrt{\mathcal{N}}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}, \tag{A5}$$

with the summation convention implied over repeated indices and for any pairs $a, a' = 1, \cdots, N$ or $\boldsymbol{R}, \boldsymbol{R}' \in \Lambda_R$ or $\boldsymbol{k}, \boldsymbol{k}' \in \Lambda^\star_{\text{BZ}}$.

The orbital and band basis in momentum space are related by the momentum resolved $N \times N$ unitary matrix $U_{\boldsymbol{k}}$ with the matrix elements

$$\langle \psi^\alpha_{\boldsymbol{k}}|\chi^a_{\boldsymbol{k}}\rangle = u^{\alpha a}_{\boldsymbol{k}}, \qquad \alpha, a = 1, \cdots, N. \tag{A6a}$$

Hence, for any $\boldsymbol{k} \in \Lambda^\star_{\text{BZ}}$, these matrix elements obey the orthonormality conditions

$$u^{\alpha a}_{\boldsymbol{k}}\, u^{\alpha' a *}_{\boldsymbol{k}} = \delta^{\alpha,\alpha'}, \qquad \alpha, \alpha' = 1, \cdots, N, \tag{A6b}$$

for row multiplication or

$$u^{\alpha a *}_{\boldsymbol{k}}\, u^{\alpha a'}_{\boldsymbol{k}} = \delta^{a,a'}, \qquad a, a' = 1, \cdots, N, \tag{A6c}$$

for column multiplication.

The orbital basis in position space and the band basis in momentum space are related by the Fourier component

$$\langle \psi^\alpha_{\boldsymbol{r}}|\chi^a_{\boldsymbol{k}}\rangle = \frac{1}{\sqrt{\mathcal{N}}}\, u^{\alpha a}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \qquad \alpha, a = 1, \cdots, N, \tag{A7}$$

for any $\boldsymbol{r} \in \Lambda_r$ and any $\boldsymbol{k} \in \Lambda^\star_{\text{BZ}}$.

The orbital and band basis in position space are related by the convolution

$$\begin{aligned} |W^a_{\boldsymbol{R}}\rangle &= \frac{1}{\sqrt{\mathcal{N}}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\, |\chi^a_{\boldsymbol{k}}\rangle \\ &= \frac{1}{\sqrt{\mathcal{N}}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \Big(|\psi^\alpha_{\boldsymbol{r}}\rangle\langle\psi^\alpha_{\boldsymbol{r}}|\Big)|\chi^a_{\boldsymbol{k}}\rangle \\ &= \frac{1}{\sqrt{\mathcal{N}}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \Big(\langle\psi^\alpha_{\boldsymbol{r}}|\chi^a_{\boldsymbol{k}}\rangle\Big)|\psi^\alpha_{\boldsymbol{r}}\rangle \\ \text{Eq. (A7)} \qquad &= \frac{1}{\mathcal{N}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{r})}\, u^{\alpha a}_{\boldsymbol{k}}\, |\psi^\alpha_{\boldsymbol{r}}\rangle \end{aligned} \tag{A8}$$

for any $\boldsymbol{R} \in \Lambda_R$ with the summation convention over repeated indices on the right-hand side.

2. Projected lattice position operator

A lattice position operator generates infinitesimal translations in momentum space. There is an ambiguity when defining a lattice position operator. We can either choose to define the position operator on the lattice Λ_r or on the lattice Λ_R. In the former case, we define

$$\begin{aligned} \widehat{\boldsymbol{r}} &:= \sum_{\boldsymbol{r}\in\Lambda_r} \sum_{\alpha=1}^{N} |\psi^\alpha_{\boldsymbol{r}}\rangle\, \boldsymbol{r}\, \langle\psi^\alpha_{\boldsymbol{r}}| \\ &\equiv |\psi^\alpha_{\boldsymbol{r}}\rangle\, \boldsymbol{r}\, \langle\psi^\alpha_{\boldsymbol{r}}| \end{aligned} \tag{A9}$$

with the summation convention over the repeated indices $\alpha = 1, \cdots, N$ and $\boldsymbol{r} \in \Lambda_r$ implied on the second line. In the latter case, we define

$$\begin{aligned} \widehat{\boldsymbol{R}} &:= \sum_{\boldsymbol{R}\in\Lambda_R} \sum_{a=1}^{N} |W^a_{\boldsymbol{R}}\rangle\, \boldsymbol{R}\, \langle W^a_{\boldsymbol{R}}| \\ &= |W^a_{\boldsymbol{R}}\rangle\, \boldsymbol{R}\, \langle W^a_{\boldsymbol{R}}| \end{aligned} \tag{A10}$$

with the summation convention over the repeated indices $a = 1, \cdots, N$ and $\boldsymbol{R} \in \Lambda_R$ implied on the second line.

We define the projection operator on the first $\widetilde{N}$ occupied bands by

$$\begin{aligned} \widehat{p}_{\widetilde{N}} &:= \sum_{\boldsymbol{k} \in \Lambda^\star_{\mathrm{BZ}}} \sum_{\tilde{a}=1}^{\widetilde{N}} |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle \langle \chi^{\tilde{a}}_{\boldsymbol{k}}| \\ &\equiv |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle \langle \chi^{\tilde{a}}_{\boldsymbol{k}}| \end{aligned} \tag{A11}$$

with the summation convention over the repeated indices $\tilde{a} = 1, \cdots, \widetilde{N}$ and $\boldsymbol{k} \in \Lambda^\star_{\mathrm{BZ}}$ implied on the second line. In the sequel, it will always be understood that latin indices such as $\tilde{a}$ run over the first $\widetilde{N}$ occupied bands. The projection operator on the first $\widetilde{N}$ occupied bands is represented by

$$\begin{aligned} \widehat{p}_{\widetilde{N}} &= \frac{1}{\mathcal{N}} \sum_{\boldsymbol{k} \in \Lambda^\star_{\mathrm{BZ}}} e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')} |W^{\tilde{a}}_{\boldsymbol{R}}\rangle\langle W^{\tilde{a}}_{\boldsymbol{R}'}| \\ &= |W^{\tilde{a}}_{\boldsymbol{R}}\rangle\langle W^{\tilde{a}}_{\boldsymbol{R}}| \end{aligned} \tag{A12}$$

in the Wannier basis (with the summation convention over the repeated indices $\tilde{a} = 1, \cdots, \widetilde{N}$ and $\boldsymbol{R} \in \Lambda_R$ on the second line). The projection operator on the first $\widetilde{N}$ occupied bands is represented by

$$\widehat{p}_{\widetilde{N}} = u^{\alpha\tilde{a}}_{\boldsymbol{k}}\, u^{\alpha'\tilde{a}*}_{\boldsymbol{k}}\, |\psi^{\alpha}_{\boldsymbol{k}}\rangle\langle\psi^{\alpha'}_{\boldsymbol{k}}| \tag{A13}$$

in the momentum space orbital basis (with the summation convention over the repeated indices $\tilde{a} = 1, \cdots, \widetilde{N}$, $\alpha, \alpha' = 1, \cdots, N$, and $\boldsymbol{k} \in \Lambda^\star_{\mathrm{BZ}}$). It is not diagonal in the orbital indices because of the truncation to the occupied band.

The lattice position operator projected on the first $\widetilde{N}$ occupied bands can be either defined by

$$\widehat{\boldsymbol{X}}_r := \widehat{p}_{\widetilde{N}}\, \hat{\boldsymbol{r}}\, \widehat{p}_{\widetilde{N}} \tag{A14}$$

or by

$$\widehat{\boldsymbol{X}}_R := \widehat{p}_{\widetilde{N}}\, \hat{\boldsymbol{R}}\, \widehat{p}_{\widetilde{N}}. \tag{A15}$$

3. Lattice discretization of the single-particle trace over the 1-bracket of the projected position operator

We are first going to show that

$$\mathrm{Tr}\, \left(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R \right) = \sum_{\tilde{a}=1}^{\widetilde{N}} \left(\sum_{\boldsymbol{r} \in \Lambda_r} \boldsymbol{r} - \sum_{\boldsymbol{R} \in \Lambda_R} \boldsymbol{R} \right). \tag{A16}$$

We are then going to show that

$$\mathrm{Tr}\, \left(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R \right) = \mathrm{i} \sum_{\boldsymbol{k} \in \Lambda^\star_{\mathrm{BZ}}} \mathrm{tr}\, \boldsymbol{A}_{\boldsymbol{k}} \tag{A17a}$$

where, in the thermodynamic limit $\mathcal{N} \to \infty$ and assuming smoothness of the $\boldsymbol{k}$ dependence of the matrix elements (A6a), $\boldsymbol{A}_{\boldsymbol{k}}$ is the $\widetilde{N} \times \widetilde{N}$ antisymmetric matrix with the components

$$\boldsymbol{A}^{\tilde{a}\tilde{b}}_{\boldsymbol{k}} := u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, \partial_{\boldsymbol{k}}\, u^{\alpha\tilde{b}}_{\boldsymbol{k}}, \qquad \tilde{a}, \tilde{b} = 1, \cdots, \widetilde{N}. \tag{A17b}$$

The summation convention over repeated indices is implied. Comments: (i) Equation (A17) follows from the identity (the proof of which is postponed to Sec. A 5)

$$\widehat{\boldsymbol{X}}_r = \widehat{\boldsymbol{X}}_R + |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle\, \mathrm{i}\, \boldsymbol{A}^{\tilde{a}\tilde{b}}_{\boldsymbol{k}}\, \langle \chi^{\tilde{b}}_{\boldsymbol{k}}|. \tag{A18}$$

(ii) Equation (A17) holds for any choice of the boundary conditions. (iii) Equation (A16) is mathematically meaningless in the thermodynamic limit $\mathcal{N} \to \infty$, for it involves the subtraction of two ill-conditioned sums.

Proof. First, we make two observations. On the one hand, from the definition (A14)

$$\begin{aligned}
\operatorname{Tr}\widehat{\boldsymbol{X}}_r &= \langle W^a_{\boldsymbol{R}}|\,\widehat{\boldsymbol{X}}_r\,|W^a_{\boldsymbol{R}}\rangle \\
&\overset{\text{Eqs. (A14) and (A12)}}{=} \langle W^{\tilde{a}}_{\boldsymbol{R}}|\,\hat{\boldsymbol{r}}\,|W^{\tilde{a}}_{\boldsymbol{R}}\rangle \\
&\overset{\text{Eq. (A8)}}{=} \left[\frac{1}{\mathcal{N}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{r})}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,\langle\psi^{\alpha}_{\boldsymbol{r}}|\right]\,\hat{\boldsymbol{r}}\left[\frac{1}{\mathcal{N}}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{R}-\boldsymbol{r}')}\,u^{\alpha'\tilde{a}}_{\boldsymbol{k}'}\,|\psi^{\alpha'}_{\boldsymbol{r}'}\rangle\right] \\
&\overset{\text{Eq. (A9)}}{=} \left[\frac{1}{\mathcal{N}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{r})}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,\langle\psi^{\alpha}_{\boldsymbol{r}}|\right]\,\boldsymbol{r}\left[\frac{1}{\mathcal{N}}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{R}-\boldsymbol{r}')}\,u^{\alpha'\tilde{a}}_{\boldsymbol{k}'}\,|\psi^{\alpha'}_{\boldsymbol{r}'}\rangle\right] \\
&\overset{\langle\psi^{\alpha}_{\boldsymbol{r}}|\psi^{\alpha'}_{\boldsymbol{r}'}\rangle=\delta^{\alpha,\alpha'}\delta_{\boldsymbol{r},\boldsymbol{r}'}}{=} \sum_{\boldsymbol{r}\in\Lambda_r}\left[\frac{1}{\mathcal{N}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\right]\,\boldsymbol{r}\left[\frac{1}{\mathcal{N}}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}}\,u^{\alpha\tilde{a}}_{\boldsymbol{k}'}\right].
\end{aligned} \tag{A19}$$

The implied summation over $\boldsymbol{R}$ produces the factor $\mathcal{N}\,\delta_{\boldsymbol{k},\boldsymbol{k}'}$. We are left with the implied summations over the orbital $\alpha = 1,\cdots,N$, over the occupied bands $\tilde{a} = 1,\cdots,\widetilde{N}$, and over the momenta $\boldsymbol{k}\in\Lambda^{\star}_{\mathrm{BZ}}$,

$$\begin{aligned}
\operatorname{Tr}\widehat{\boldsymbol{X}}_r &= \frac{1}{\mathcal{N}}\,\left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,u^{\alpha\tilde{a}}_{\boldsymbol{k}}\right)\sum_{\boldsymbol{r}\in\Lambda_r}\boldsymbol{r} \\
&\overset{\text{Eqs. (A6b) and (A6c)}}{=} \sum_{\tilde{a}=1}^{\widetilde{N}}\sum_{\boldsymbol{r}\in\Lambda_r}\boldsymbol{r}.
\end{aligned} \tag{A20}$$

On the other hand, the definition (A15) immediately implies that

$$\begin{aligned}
\operatorname{Tr}\widehat{\boldsymbol{X}}_R &= \langle W^a_{\boldsymbol{R}}|\,\widehat{\boldsymbol{X}}_R\,|W^a_{\boldsymbol{R}}\rangle \\
&\overset{\text{Eqs. (A15) and (A12)}}{=} \langle W^{\tilde{a}}_{\boldsymbol{R}}|\,\hat{\boldsymbol{R}}\,|W^{\tilde{a}}_{\boldsymbol{R}}\rangle \\
&= \sum_{\tilde{a}=1}^{\widetilde{N}}\sum_{\boldsymbol{R}\in\Lambda_r}\boldsymbol{R}.
\end{aligned} \tag{A21}$$

Subtracting Eq. (A21) from Eq. (A20) delivers Eq. (A16).

Second, to prove Eq. (A17), we start from Eqs. (A14) and (A11) to establish that

$$\begin{aligned}
\operatorname{Tr}\widehat{\boldsymbol{X}}_r &= \langle\chi^a_{\boldsymbol{k}}|\,\widehat{\boldsymbol{X}}_r\,|\chi^a_{\boldsymbol{k}}\rangle \\
&\overset{\text{Eqs. (A14) and (A11)}}{=} \langle\chi^{\tilde{a}}_{\boldsymbol{k}}|\,\hat{\boldsymbol{r}}\,|\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle \\
&= \langle\chi^{\tilde{a}}_{\boldsymbol{k}}|\left(|\psi^{\alpha}_{\boldsymbol{r}}\rangle\langle\psi^{\alpha}_{\boldsymbol{r}}|\right)\hat{\boldsymbol{r}}\,|\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle \\
&\overset{\text{Eq. (A9)}}{=} \left(\langle\chi^{\tilde{a}}_{\boldsymbol{k}}|\psi^{\alpha}_{\boldsymbol{r}}\rangle\right)\left(\boldsymbol{r}\,\langle\psi^{\alpha}_{\boldsymbol{r}}|\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle\right) \\
&\overset{\text{Eq. (A7)}}{=} \left(\langle\chi^{\tilde{a}}_{\boldsymbol{k}}|\psi^{\alpha}_{\boldsymbol{r}}\rangle\right)\left(\boldsymbol{r}\,\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}}\,u^{\alpha\tilde{a}}_{\boldsymbol{k}}\right) \\
&= \left(\langle\chi^{\tilde{a}}_{\boldsymbol{k}}|\psi^{\alpha}_{\boldsymbol{r}}\rangle\right)\left[\left(-\mathrm{i}\partial_{\boldsymbol{k}}\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}}\right)u^{\alpha\tilde{a}}_{\boldsymbol{k}}\right] \\
&= \left(\frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\right)\left[(-\mathrm{i})\partial_{\boldsymbol{k}}\left(\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}}u^{\alpha\tilde{a}}_{\boldsymbol{k}}\right)-\left(\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}}(-\mathrm{i})\partial_{\boldsymbol{k}}u^{\alpha\tilde{a}}_{\boldsymbol{k}}\right)\right] \\
&= \langle\chi^{\tilde{a}}_{\boldsymbol{k}}|\psi^{\alpha}_{\boldsymbol{r}}\rangle(-\mathrm{i})\partial_{\boldsymbol{k}}\langle\psi^{\alpha}_{\boldsymbol{r}}|\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle+\mathrm{i}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\partial_{\boldsymbol{k}}u^{\alpha\tilde{a}}_{\boldsymbol{k}}.
\end{aligned} \tag{A22}$$

To prove Eq. (A17), it suffices to recognize that

$$\mathrm{i}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\partial_{\boldsymbol{k}}u^{\alpha\tilde{a}}_{\boldsymbol{k}} = \sum_{\boldsymbol{k}\in\Lambda^{\star}_{\mathrm{BZ}}}\mathrm{i}\operatorname{tr}\boldsymbol{A}_{\boldsymbol{k}} \tag{A23}$$

and that, after insertion of the Fourier expansion within the band basis (A5),

$$\begin{aligned}
\langle\chi^{\tilde{a}}_{\boldsymbol{k}}|\psi^{\alpha}_{\boldsymbol{r}}\rangle(-\mathrm{i})\partial_{\boldsymbol{k}}\langle\psi^{\alpha}_{\boldsymbol{r}}|\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle &= \left(\frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'}}{\sqrt{\mathcal{N}}}\langle W^{\tilde{a}}_{\boldsymbol{R}'}|\psi^{\alpha}_{\boldsymbol{r}}\rangle\right)(-\mathrm{i})\,\partial_{\boldsymbol{k}}\left(\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}}\langle\psi^{\alpha}_{\boldsymbol{r}}|W^{\tilde{a}}_{\boldsymbol{R}}\rangle\right)\\
&= \left(\frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'}}{\sqrt{\mathcal{N}}}\langle W^{\tilde{a}}_{\boldsymbol{R}'}|\psi^{\alpha}_{\boldsymbol{r}}\rangle\right)\left(\boldsymbol{R}\,\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}}\langle\psi^{\alpha}_{\boldsymbol{r}}|W^{\tilde{a}}_{\boldsymbol{R}}\rangle\right)\\
&= \left(\sum_{\boldsymbol{k}\in\Lambda^{\star}_{\mathrm{BZ}}}\frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\left(\boldsymbol{R}'-\boldsymbol{R}\right)}}{\mathcal{N}}\right)\langle W^{\tilde{a}}_{\boldsymbol{R}'}|\boldsymbol{R}\left(|\psi^{\alpha}_{\boldsymbol{r}}\rangle\langle\psi^{\alpha}_{\boldsymbol{r}}\right)|W^{\tilde{a}}_{\boldsymbol{R}}\rangle\\
&= \langle W^{\tilde{a}}_{\boldsymbol{R}}|\boldsymbol{R}\,|W^{\tilde{a}}_{\boldsymbol{R}}\rangle\\
&= \mathrm{Tr}\,\widehat{\boldsymbol{X}}_{R}.
\end{aligned} \tag{A24}$$

□

4. Lattice discretization of the 2-bracket of the projected position operator

We are going to establish that the 2-bracket of the projected positions operator (A14) is

$$\begin{aligned}
\epsilon_{\mu\nu}\,\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r} &= |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle\,\left(-F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}}\right)\,\langle\chi^{\tilde{b}}_{\boldsymbol{k}}|\\
&= |W^{\tilde{a}}_{\boldsymbol{R}}\rangle\,\left(-\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\,F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}}\right)\,\langle W^{\tilde{b}}_{\boldsymbol{R}'}|
\end{aligned} \tag{A25a}$$

where

$$F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}} = \partial_{\mu}\,A^{\tilde{a}\tilde{b}}_{\boldsymbol{k};\nu} - \partial_{\nu}\,A^{\tilde{a}\tilde{b}}_{\boldsymbol{k};\mu} + \left[A_{\boldsymbol{k};\mu},A_{\boldsymbol{k};\nu}\right]^{\tilde{a}\tilde{b}},\qquad \tilde{a},\tilde{b}=1,\cdots,\widetilde{N},\qquad \boldsymbol{k}\in\Lambda^{\star}_{\mathrm{BZ}}, \tag{A25b}$$

in the thermodynamic limit $\mathcal{N}\to\infty$ and assuming smoothness of the $\boldsymbol{k}$ dependence of the matrix elements (A6a). The summation convention over repeated indices is implied. In contrast, the 2-bracket of the projected positions operator (A15) vanishes

$$\epsilon_{\mu\nu}\,\widehat{X}^{\mu}_{R}\,\widehat{X}^{\nu}_{R} = 0. \tag{A26}$$

Comments: (i) No regularization is needed here. (ii) Equation (A25) holds for any choice of the boundary conditions.

Proof. We begin with the proof of Eq. (A25) which we establish by computing the matrix elements of $\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}$ in the band basis (A5) in the Wannier representation (as opposed to the momentum representation). For any triplet of pairs $a,a'=1,\cdots,N$, $\boldsymbol{R},\boldsymbol{R}'\in\Lambda_R$, and $\mu,\nu=1,\cdots,d$, we evaluate the matrix element of $\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}$ in the Wannier basis given by

$$\begin{aligned}
\langle W^{a}_{\boldsymbol{R}}|\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}\,|W^{a'}_{\boldsymbol{R}'}\rangle &= \langle W^{a}_{\boldsymbol{R}}|\left(\widehat{p}_{\widetilde{N}}\,\hat{r}^{\mu}\,\widehat{p}_{\widetilde{N}}\right)\left(\widehat{p}_{\widetilde{N}}\hat{r}^{\nu}\,\widehat{p}_{\widetilde{N}}\right)\,|W^{a'}_{\boldsymbol{R}'}\rangle\\
&= \delta^{a,\tilde{a}}\times\delta^{a',\tilde{a}'}\times\langle W^{\tilde{a}}_{\boldsymbol{R}}|\,\hat{r}^{\mu}\,\widehat{p}_{\widetilde{N}}\,\hat{r}^{\nu}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle.
\end{aligned} \tag{A27}$$

With the help of Eqs. (A4) and (A5),

$$\begin{aligned}
\langle W^{\tilde{a}}_{\boldsymbol{R}}|\,\hat{r}^{\mu}\,\widehat{p}_{\widetilde{N}}\,\hat{r}^{\nu}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle &= \langle W^{\tilde{a}}_{\boldsymbol{R}}|\,\left(|\psi^{\alpha}_{\boldsymbol{r}}\rangle\langle\psi^{\alpha}_{\boldsymbol{r}}|\right)\hat{r}^{\mu}\,\left(|\chi^{\tilde{b}}_{\boldsymbol{p}}\rangle\langle\chi^{\tilde{b}}_{\boldsymbol{p}}|\right)\hat{r}^{\nu}\,\left(|\psi^{\alpha'}_{\boldsymbol{r}'}\rangle\langle\psi^{\alpha'}_{\boldsymbol{r}'}|\right)|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle\\
&\overset{\text{Eq. (A9)}}{=} r^{\mu}\,r'^{\nu}\,\langle W^{\tilde{a}}_{\boldsymbol{R}}|\psi^{\alpha}_{\boldsymbol{r}}\rangle\times\langle\psi^{\alpha}_{\boldsymbol{r}}|\chi^{\tilde{b}}_{\boldsymbol{p}}\rangle\times\langle\chi^{\tilde{b}}_{\boldsymbol{p}}|\psi^{\alpha'}_{\boldsymbol{r}'}\rangle\times\langle\psi^{\alpha'}_{\boldsymbol{r}'}|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle\\
&\overset{\text{Eqs. (A7)+(A8)}}{=} \frac{1}{\mathcal{N}^3}r^{\mu}\,r'^{\nu}\,\left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{r})}\right)\times\left(u^{\alpha\tilde{b}}_{\boldsymbol{p}}\,e^{+\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\right)\times\left(u^{\alpha'\tilde{b}*}_{\boldsymbol{p}}\,e^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}'}\right)\times\left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{R}'-\boldsymbol{r}')}\right)\\
&= \frac{1}{\mathcal{N}^3}\left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\,\frac{\partial}{\partial k^{\mu}}e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}\right)\times\left(u^{\alpha\tilde{b}}_{\boldsymbol{p}}\,e^{+\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}}\right)\times\left(u^{\alpha'\tilde{b}*}_{\boldsymbol{p}}\,e^{-\mathrm{i}\boldsymbol{p}\cdot\boldsymbol{r}'}\right)\times\left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\,\frac{\partial}{\partial k'^{\nu}}\,e^{+\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{r}'}\right).
\end{aligned} \tag{A28}$$

We would like to perform the implicit sums over $\boldsymbol{r} \in \Lambda_r$ and $\boldsymbol{r}' \in \Lambda_r$. To this end we use twice the product rule for differentiation,

$$\begin{aligned} f(\partial g) f'(\partial' g') &= [\partial(fg) - (\partial f) g]\,[\partial'(f'g') - (\partial' f') g'] \\ &= \partial(fg)\partial'(f'g') - \partial(fg)(\partial' f') g' - (\partial f) g \partial'(f'g') + (\partial f) g (\partial' f') g' \\ &= \partial\partial'(fgf'g') - \partial[fg(\partial' f') g'] - \partial'[(\partial f) g f' g'] + (\partial f) g (\partial' f) g' \end{aligned} \tag{A29}$$

for any pair of functions f and g of one variable and for any pair of functions f' and g' of another independent variable. We find

$$\begin{aligned} \langle W^{\tilde{a}}_{\boldsymbol{R}} | \widehat{X}^{\mu}_{r}\, \widehat{X}^{\nu}_{r} \, | W^{\tilde{a}'}_{\boldsymbol{R}'} \rangle = &+ \frac{1}{\mathcal{N}^3} \frac{\partial}{\partial k^{\mu}} \frac{\partial}{\partial k'^{\nu}} \left[\left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \times \left(u^{\alpha\tilde{b}}_{\boldsymbol{p}}\, e^{+\mathrm{i}(\boldsymbol{p}-\boldsymbol{k})\cdot\boldsymbol{r}} \right) \times \left(u^{\alpha'\tilde{b}*}_{\boldsymbol{p}}\, e^{-\mathrm{i}(\boldsymbol{p}-\boldsymbol{k}')\cdot\boldsymbol{r}'} \right) \times \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right] \\ &- \frac{1}{\mathcal{N}^3} \frac{\partial}{\partial k^{\mu}} \left\{ \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \times \left(u^{\alpha\tilde{b}}_{\boldsymbol{p}}\, e^{+\mathrm{i}(\boldsymbol{p}-\boldsymbol{k})\cdot\boldsymbol{r}} \right) \times \left(u^{\alpha'\tilde{b}*}_{\boldsymbol{p}}\, e^{-\mathrm{i}(\boldsymbol{p}-\boldsymbol{k}')\cdot\boldsymbol{r}'} \right) \times \left[\partial'_{\nu} \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right] \right\} \\ &- \frac{1}{\mathcal{N}^3} \frac{\partial}{\partial k'^{\nu}} \left\{ \left[\partial_{\mu} \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \right] \times \left(u^{\alpha\tilde{b}}_{\boldsymbol{p}}\, e^{+\mathrm{i}(\boldsymbol{p}-\boldsymbol{k})\cdot\boldsymbol{r}} \right) \times \left(u^{\alpha'\tilde{b}*}_{\boldsymbol{p}}\, e^{-\mathrm{i}(\boldsymbol{p}-\boldsymbol{k}')\cdot\boldsymbol{r}'} \right) \times \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right\} \\ &+ \frac{1}{\mathcal{N}^3} \left[\partial_{\mu} \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \right] \times \left(u^{\alpha\tilde{b}}_{\boldsymbol{p}}\, e^{+\mathrm{i}(\boldsymbol{p}-\boldsymbol{k})\cdot\boldsymbol{r}} \right) \times \left(u^{\alpha'\tilde{b}*}_{\boldsymbol{p}}\, e^{-\mathrm{i}(\boldsymbol{p}-\boldsymbol{k}')\cdot\boldsymbol{r}'} \right) \times \left[\partial'_{\nu} \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right]. \end{aligned} \tag{A30}$$

We perform the implicit sum over $\boldsymbol{r} \in \Lambda_r$ on lines 1 and 2. We perform the implicit sum over $\boldsymbol{r}' \in \Lambda_r$ on line 3. We perform the implicit sum over the pair $\boldsymbol{r}, \boldsymbol{r}' \in \Lambda_r$ on line 4. The implicit sum over $\boldsymbol{r} \in \Lambda_r$ yields the multiplicative factor $\mathcal{N}\delta_{\boldsymbol{k},\boldsymbol{p}}$, while the implicit sum over $\boldsymbol{r}' \in \Lambda_r$ yields the multiplicative factor $\mathcal{N}\delta_{\boldsymbol{k}',\boldsymbol{p}}$. Thus,

$$\begin{aligned} \langle W^{\tilde{a}}_{\boldsymbol{R}} | \widehat{X}^{\mu}_{r}\, \widehat{X}^{\nu}_{r} \, | W^{\tilde{a}'}_{\boldsymbol{R}'} \rangle = &+ \frac{1}{\mathcal{N}^2} \frac{\partial}{\partial k^{\mu}} \frac{\partial}{\partial k'^{\nu}} \left[\left(e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \delta^{\tilde{a}\tilde{b}} \right) \times \left(u^{\alpha'\tilde{b}*}_{\boldsymbol{k}}\, e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}'} \right) \times \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right] \\ &- \frac{1}{\mathcal{N}^2} \frac{\partial}{\partial k^{\mu}} \left\{ \left(e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \delta^{\tilde{a}\tilde{b}} \right) \times \left(u^{\alpha'\tilde{b}*}_{\boldsymbol{k}}\, e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}'} \right) \times \left[\partial'_{\nu} \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'} e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right] \right\} \\ &- \frac{1}{\mathcal{N}^2} \frac{\partial}{\partial k'^{\nu}} \left\{ \left[\partial_{\mu} \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \right] \times \left(u^{\alpha\tilde{b}}_{\boldsymbol{k}'}\, e^{+\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{r}} \right) \times \left(\delta^{\tilde{b}\tilde{a}'} e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right\} \\ &+ \frac{1}{\mathcal{N}} \left\{ \left[\partial_{\mu} \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \right] u^{\alpha\tilde{b}}_{\boldsymbol{k}} \right\} \times \left\{ \left[u^{\alpha'\tilde{b}*}_{\boldsymbol{k}}\, \partial_{\nu} \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'} \right) \right] \right\}. \end{aligned} \tag{A31}$$

Performing the implicit sum over the projected band index $\tilde{b} = 1, \cdots, \widetilde{N}$ on lines 1, 2, and 3 gives

$$\begin{aligned} \langle W^{\tilde{a}}_{\boldsymbol{R}} | \widehat{X}^{\mu}_{r}\, \widehat{X}^{\nu}_{r} \, | W^{\tilde{a}'}_{\boldsymbol{R}'} \rangle = &+ \frac{1}{\mathcal{N}^2} \frac{\partial}{\partial k^{\mu}} \frac{\partial}{\partial k'^{\nu}} \left[u^{\alpha'\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \times e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \times u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right] \\ &- \frac{1}{\mathcal{N}^2} \frac{\partial}{\partial k^{\mu}} \left\{ u^{\alpha'\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \times e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \times \left[\partial'_{\nu} u^{\alpha'\tilde{a}'}_{\boldsymbol{k}'} e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right] \right\} \\ &- \frac{1}{\mathcal{N}^2} \frac{\partial}{\partial k'^{\nu}} \left\{ \left[\partial_{\mu} u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right] \times e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \times u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right\} \\ &+ \frac{1}{\mathcal{N}} \left\{ \left[\partial_{\mu} \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \right] u^{\alpha\tilde{b}}_{\boldsymbol{k}} \right\} \times \left\{ \left[u^{\alpha'\tilde{b}*}_{\boldsymbol{k}}\, \partial_{\nu} \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'} \right) \right] \right\}. \end{aligned} \tag{A32}$$

For further simplification, we apply the identity

$$\begin{aligned} \underline{\partial_k \partial_{k'} \left[f(k)\, h(k,k')\, g(k') \right]} = &+ \underline{\partial_k \left[f(k)\, h(k,k')\, \partial_{k'} g(k') \right]} \\ &+ \underline{\partial_{k'} \left[g(k')\, h(k,k')\, \partial_k f(k) \right]} \\ &+ f(k)\, g(k')\, \partial_k \partial_{k'} h(k,k') \\ &- h(k,k')\, \left[\partial_k f(k) \right] \left[\partial_k g(k') \right] \end{aligned} \tag{A33}$$

for the smooth function f, g, and h to the first three lines of Eq. (A32). We find

$$\begin{aligned} \langle W^{\tilde{a}}_{\boldsymbol{R}} | \widehat{X}^{\mu}_{r}\, \widehat{X}^{\nu}_{r} \, | W^{\tilde{a}'}_{\boldsymbol{R}'} \rangle = &+ \frac{1}{\mathcal{N}^2} \left[\frac{\partial}{\partial k^{\mu}} \frac{\partial}{\partial k'^{\nu}} e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \right] \times u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \times u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\, e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \\ &- \frac{1}{\mathcal{N}^2}\, e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}} \left[\partial_{\mu} \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \right] \times \left[\partial'_{\nu} \left(u^{\alpha\tilde{a}'}_{\boldsymbol{k}'} e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'} \right) \right] \\ &+ \frac{1}{\mathcal{N}} \left[\partial_{\mu} \left(u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\, e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}} \right) \right] u^{\alpha\tilde{b}}_{\boldsymbol{k}} \times \left[u^{\alpha'\tilde{b}*}_{\boldsymbol{k}}\, \partial_{\nu} \left(u^{\alpha'\tilde{a}'}_{\boldsymbol{k}}\, e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'} \right) \right]. \end{aligned} \tag{A34}$$

We perform the derivatives on lines 2 and 3 first, which we then follow up with the implicit sum over $\boldsymbol{r}$,

$$\begin{aligned}\langle W^{\tilde{a}}_{\boldsymbol{R}}|\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle = &+\frac{1}{\mathcal{N}^2}\left[\frac{\partial}{\partial k^{\mu}}\frac{\partial}{\partial k'^{\nu}}e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}\right]\times u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\times u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\\ &-\frac{1}{\mathcal{N}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}\left[\mathrm{i}R_{\mu}u^{\alpha\tilde{a}*}_{\boldsymbol{k}}+\partial_{\mu}u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\right]\times\left[-\mathrm{i}R'_{\nu}u^{\alpha\tilde{a}'}_{\boldsymbol{k}}+\partial'_{\nu}u^{\alpha\tilde{a}'}_{\boldsymbol{k}}\right]\\ &+\frac{1}{\mathcal{N}}e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}\left[\mathrm{i}R_{\mu}u^{\alpha\tilde{a}*}_{\boldsymbol{k}}+\partial_{\mu}u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\right]u^{\alpha\tilde{b}}_{\boldsymbol{k}}\times u^{\alpha'\tilde{b}*}_{\boldsymbol{k}}\left[-\mathrm{i}R'_{\nu}u^{\alpha'\tilde{a}'}_{\boldsymbol{k}}+\partial_{\nu}u^{\alpha'\tilde{a}'}_{\boldsymbol{k}}\right].\end{aligned}\tag{A35}$$

By making use of the orthonormality (A6b) and (A6c) and the definition (A17b) for the gauge connection, we can expand the product of the bracketed terms on line 2 and 3 according to

$$\begin{aligned}\langle W^{\tilde{a}}_{\boldsymbol{R}}|\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle = &+\frac{1}{\mathcal{N}^2}\left[\frac{\partial}{\partial k^{\mu}}\frac{\partial}{\partial k'^{\nu}}e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}\right]\times u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\times u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\\ &-\frac{e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\left[\underline{R_{\mu}\,R'_{\nu}\,\delta^{\tilde{a}\tilde{a}'}+\mathrm{i}\,R_{\mu}\,A^{\tilde{a}\tilde{a}'}_{\nu;\boldsymbol{k}}+\mathrm{i}\,R'_{\nu}\,A^{\tilde{a}\tilde{a}'}_{\mu;\boldsymbol{k}}}+\left(\partial_{\mu}u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\right)\left(\partial_{\nu}u^{\alpha\tilde{a}'}_{\boldsymbol{k}}\right)\right]\\ &+\frac{e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\left(\mathrm{i}R_{\mu}\delta^{\tilde{a}\tilde{b}}-A^{\tilde{a}\tilde{b}}_{\mu;\boldsymbol{k}}\right)\times\left(-\mathrm{i}R'_{\nu}\delta^{\tilde{b}\tilde{a}'}+A^{\tilde{b}\tilde{a}'}_{\nu;\boldsymbol{k}}\right).\end{aligned}\tag{A36}$$

Terms that have been underlined on line 2 cancel with line 3, leaving us with

$$\begin{aligned}\langle W^{\tilde{a}}_{\boldsymbol{R}}|\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle = &+\frac{1}{\mathcal{N}^2}\left[\frac{\partial}{\partial k^{\mu}}\frac{\partial}{\partial k'^{\nu}}e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}\right]\times u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}\times u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\,e^{-\mathrm{i}\boldsymbol{k}'\cdot\boldsymbol{R}'}\\ &-\frac{e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\left[\left(\partial_{\mu}u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\right)\left(\partial_{\nu}u^{\alpha\tilde{a}'}_{\boldsymbol{k}}\right)+A^{\tilde{a}\tilde{b}}_{\mu;\boldsymbol{k}}\,A^{\tilde{b}\tilde{a}'}_{\nu;\boldsymbol{k}}\right].\end{aligned}\tag{A37}$$

Here we would have to stop if we do not want to anti-symmetrize the indices $\mu=1,\cdots,d$ and $\nu=1,\cdots$; doing so, however, yields

$$\begin{aligned}\epsilon_{\mu\nu}\,\langle W^{\tilde{a}}_{\boldsymbol{R}}|\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle &= -\frac{e^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\left[\epsilon_{\mu\nu}\epsilon_{\mu\nu}\partial_{\mu}A^{\tilde{b}\tilde{a}'}_{\nu;\boldsymbol{k}}+A^{\tilde{a}\tilde{b}}_{\mu;\boldsymbol{k}}\,A^{\tilde{b}\tilde{a}'}_{\nu;\boldsymbol{k}}\right]\\ &= -\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\,F^{\tilde{a}\tilde{a}'}_{\mu\nu;\boldsymbol{k}}.\end{aligned}\tag{A38}$$

We continue with the proof of Eq. (A26), which we establish by computing the matrix elements of $\widehat{X}^{\mu}_{r}\,\widehat{X}^{\nu}_{r}$ in the projected band basis (A5) in the Wannier representation (as opposed to the momentum representation). For any triplet of pair $a,a'=1,\cdots,N$, $\boldsymbol{R},\boldsymbol{R}'\in\Lambda_R$, and $\mu,\nu=1,\cdots,d$, we evaluate the matrix element of $\widehat{X}^{\mu}_{R}\,\widehat{X}^{\nu}_{R}$ in the Wannier basis given by

$$\begin{aligned}\langle W^{a}_{\boldsymbol{R}}|\widehat{X}^{\mu}_{R}\,\widehat{X}^{\nu}_{R}\,|W^{a'}_{\boldsymbol{R}'}\rangle &= \delta^{a,\tilde{a}}\times\delta^{a',\tilde{a}'}\times\langle W^{a}_{\boldsymbol{R}}|\left(\widehat{p}_{\widetilde{N}}\,\hat{R}^{\mu}\,\widehat{p}_{\widetilde{N}}\right)\left(p_{\widetilde{N}}\hat{R}^{\nu}\,p_{\widetilde{N}}\right)|W^{a'}_{\boldsymbol{R}'}\rangle\\ &= \delta^{a,\tilde{a}}\times\delta^{a',\tilde{a}'}\times\langle W^{\tilde{a}}_{\boldsymbol{R}}|\,\hat{R}^{\mu}\;p_{\widetilde{N}}\,\hat{R}^{\nu}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle\\ &= \delta^{a,\tilde{a}}\times\delta^{a',\tilde{a}'}\times\langle W^{\tilde{a}}_{\boldsymbol{R}}|\,\hat{R}^{\mu}\;\left(|W^{\tilde{a}''}_{\boldsymbol{R}''}\rangle\langle W^{\tilde{a}''}_{\boldsymbol{R}''}|\right)\hat{R}^{\nu}\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle\\ &\overset{\text{Eq. (A10)}}{=} \delta^{a,\tilde{a}}\times\delta^{a',\tilde{a}'}\times R^{\mu}\,R^{\nu}\,\langle W^{\tilde{a}}_{\boldsymbol{R}}|W^{\tilde{a}''}_{\boldsymbol{R}''}\rangle\langle W^{\tilde{a}''}_{\boldsymbol{R}''}|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle\\ &= \delta^{a,\tilde{a}}\times\delta^{a',\tilde{a}'}\times R^{\mu}\,R^{\nu}\,\delta^{\tilde{a},\tilde{a}'}\,\delta_{\boldsymbol{R},\boldsymbol{R}'}.\end{aligned}\tag{A39}$$

Antisymmetrization yields Eq. (A26)

□

5. Lattice discretization of the 1- and 3-bracket of the projected position operator

We are going to show that, in the thermodynamic limit $\mathcal{N}\to\infty$ and assuming smoothness of the $\boldsymbol{k}$ dependence of the matrix elements (A6a),

$$\begin{aligned}\widehat{\boldsymbol{X}}_r &= |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle \left(\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}{\mathcal{N}}\,\boldsymbol{r}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\right)\langle\,\chi^{\tilde{a}'}_{\boldsymbol{k}'}| \\ &= |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle \left(\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}}{\mathcal{N}}\,\boldsymbol{R}\,\delta^{\tilde{a}\tilde{a}'}+\mathrm{i}\,\boldsymbol{A}^{\tilde{a}\tilde{a}'}_{\boldsymbol{k}}\,\delta_{\boldsymbol{k},\boldsymbol{k}'}\right)\langle\,\chi^{\tilde{a}'}_{\boldsymbol{k}'}| \\ &= |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle \left[\frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}'}}{\sqrt{\mathcal{N}}}\left(\delta^{\tilde{a},\tilde{a}'}\,\boldsymbol{R}'+\mathrm{i}\,\boldsymbol{A}^{\tilde{a}\tilde{a}'}_{\boldsymbol{k}}\right)\right]\langle W^{\tilde{a}'}_{\boldsymbol{R}'}| \\ &= |W^{\tilde{a}}_{\boldsymbol{R}}\rangle \left[\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\left(\delta^{\tilde{a},\tilde{a}'}\,\boldsymbol{R}'+\mathrm{i}\,\boldsymbol{A}^{\tilde{a}\tilde{a}'}_{\boldsymbol{k}}\right)\right]\langle W^{\tilde{a}'}_{\boldsymbol{R}'}|\end{aligned} \tag{A40a}$$

while

$$\epsilon_{\mu\nu\lambda}\,\widehat{X}^{\mu}_r\,\widehat{X}^{\nu}_r\,\widehat{X}^{\lambda}_r = |W^{\tilde{a}}_{\boldsymbol{R}}\rangle\left\{\frac{1}{2}\,\epsilon^{\mu\nu\lambda}\,\frac{e^{+\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}-\boldsymbol{R}')}}{\mathcal{N}}\left[(-)F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}}\left(\delta^{\tilde{b},\tilde{a}'}\,R'_{\lambda}+\mathrm{i}\,A^{\tilde{b}\tilde{a}'}_{\lambda;\boldsymbol{k}}\right)\right]\right\}\langle W^{\tilde{a}'}_{\boldsymbol{R}'}|. \tag{A40b}$$

The summation convention over repeated indices is implied. Comments: (i) A regularization is needed to dispose of the explicit $\boldsymbol{R}$ dependence in the position representation of the covariant derivative. (ii) Equation (A40) holds for any choice of the boundary conditions. The equality between the first and second right-hand side of Eq. (A40a) implies that we can do the identification

$$-\mathrm{i}\,\partial_{\boldsymbol{k}'}\left(\sum_{\boldsymbol{r}\in\Lambda_r}\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}{\mathcal{N}}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\right)+\left(\sum_{\boldsymbol{r}\in\Lambda_r}\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}{\mathcal{N}}\,u^{\alpha\tilde{a}*}_{\boldsymbol{k}}\,u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\right)\mathrm{i}\,\partial_{\boldsymbol{k}'}\longleftrightarrow\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}}{\mathcal{N}}\,\boldsymbol{R}\,\delta^{\tilde{a}\tilde{a}'} \tag{A41}$$

which will become handy to go back to a formulation in the continuum for both position and momentum that does not assume the vanishing of boundary terms. (iii) Had we chosen to represent the 3-bracket in the Bloch basis, we could have either written

$$\epsilon_{\mu\nu\lambda}\,\widehat{X}^{\mu}_r\,\widehat{X}^{\nu}_r\,\widehat{X}^{\lambda}_r = |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle\left(\frac{1}{2}\,\epsilon^{\mu\nu\lambda}\,(-)F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}}\,\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}{\mathcal{N}}\,r_{\lambda}\,u^{\alpha\tilde{b}*}_{\boldsymbol{k}}\,u^{\alpha\tilde{a}'}_{\boldsymbol{k}'}\right)\langle\chi^{\tilde{a}'}_{\boldsymbol{k}'}| \tag{A42a}$$

had we opted not to use the product rule for differentiation or

$$\epsilon_{\mu\nu\lambda}\,\widehat{X}^{\mu}_r\,\widehat{X}^{\nu}_r\,\widehat{X}^{\lambda}_r = |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle\left[\frac{1}{2}\,\epsilon^{\mu\nu\lambda}\,(-)F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}}\left(\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}}{\mathcal{N}}\,R_{\lambda}\,\delta^{\tilde{a}\tilde{a}'}+\mathrm{i}\,A^{\tilde{a}\tilde{a}'}_{\boldsymbol{k};\lambda}\,\delta_{\boldsymbol{k},\boldsymbol{k}'}\right)\right]\langle\chi^{\tilde{a}'}_{\boldsymbol{k}'}| \tag{A42b}$$

had we opted to use the product rule for differentiation. However, the representation on the first line of Eq. (A40a) as well as Eq. (A42a) are meaningless in the thermodynamic limit $\mathcal{N}\to\infty$. They fail to separate a finite and physically meaningful contribution to the trace of n-brackets.

Proof. Needed is

$$\langle W^{a}_{\boldsymbol{R}}|\left(\epsilon_{\mu\nu\lambda}\,\widehat{X}^{\mu}_r\,\widehat{X}^{\nu}_r\,\widehat{X}^{\lambda}_r\right)|W^{a'}_{\boldsymbol{R}'}\rangle=\frac{1}{2}\,\epsilon_{\mu\nu\lambda}\,\langle W^{a}_{\boldsymbol{R}}|\left(\left[\widehat{X}^{\mu}_r,\widehat{X}^{\nu}_r\right]\,\widehat{X}^{\lambda}_r\right)|W^{a'}_{\boldsymbol{R}'}\rangle \tag{A43}$$

for any pair $a,a'=1,\cdots,N$ and any pair $\boldsymbol{R},\boldsymbol{R}'\in\Lambda_R$. With the Fourier expansion within the band basis (A5) and the matrix elements (A25), there follows

$$\begin{aligned}\langle W^{a}_{\boldsymbol{R}}|\left[\widehat{X}^{\mu}_r\,,\widehat{X}^{\nu}_r\right]\,\widehat{X}^{\lambda}_r\,|W^{a'}_{\boldsymbol{R}'}\rangle &= \langle W^{a}_{\boldsymbol{R}}|\left[|\chi^{\tilde{b}}_{\boldsymbol{k}}\rangle\,\left(-F^{\tilde{b}\tilde{b}'}_{\mu\nu;\boldsymbol{k}}\right)\,\langle\chi^{\tilde{b}'}_{\boldsymbol{k}}|\right]\,\widehat{X}^{\lambda}_r\,|W^{a'}_{\boldsymbol{R}'}\rangle \\ &= \delta^{a,\tilde{a}}\times\delta^{a',\tilde{a}'}\times\langle W^{\tilde{a}}_{\boldsymbol{R}}|\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle\times\left(-F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}}\right)\times\langle\chi^{\tilde{b}}_{\boldsymbol{k}}|\widehat{X}^{\lambda}_r\,|W^{\tilde{a}'}_{\boldsymbol{R}'}\rangle\end{aligned} \tag{A44}$$

for any pair $a, a' = 1, \cdots, N$ and for any pair $\boldsymbol{R}, \boldsymbol{R}' \in \Lambda_R$. With the Fourier expansion within the band basis (A5),

$$\langle W^{a}_{\boldsymbol{R}} | \chi^{\tilde{a}}_{\boldsymbol{k}} \rangle = \delta^{a,\tilde{a}} \, \frac{e^{+\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}}. \tag{A45}$$

Equations (A40a), (A44), and (A45) imply Eq. (A40).

The proof of Eq. (A40a) is done along the same lines as in Sec. A 3. We choose the pair $a, a' = 1, \cdots, N$ and the pair $\boldsymbol{k} \in \Lambda^{\star}_{\mathrm{BZ}}$, $\boldsymbol{R} \in \Lambda_R$. With the help of Eqs. (A14) and (A11)

$$\langle \chi^{a}_{\boldsymbol{k}} | \, \widehat{\boldsymbol{X}}_r \, | W^{a'}_{\boldsymbol{R}} \rangle = \delta^{a,\tilde{a}} \times \delta^{a',\tilde{a}'} \times \langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \, \hat{\boldsymbol{r}} \, | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle. \tag{A46}$$

In turn, for any pair $\tilde{a}, \tilde{a}' = 1, \cdots, \widetilde{N}$,

$$\begin{aligned}
\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \, \hat{\boldsymbol{r}} \, | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle &= \langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \, \Big(|\psi^{\alpha}_{\boldsymbol{r}}\rangle\langle\psi^{\alpha}_{\boldsymbol{r}}| \Big) \, \hat{\boldsymbol{r}} \, | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle \\
&\overset{\text{Eq. (A9)}}{=} \Big(\boldsymbol{r} \, \langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \psi^{\alpha}_{\boldsymbol{r}} \rangle \Big) \Big(\langle \psi^{\alpha}_{\boldsymbol{r}} | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle \Big) \\
&\overset{\text{Eq. (A7) and Eq. (A8)}}{=} \Big(\boldsymbol{r} \, \frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}} u^{\alpha\tilde{a}*}_{\boldsymbol{k}} \Big) \left(\frac{e^{-\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{R}-\boldsymbol{r})}}{\mathcal{N}} \, u^{\alpha\tilde{a}'}_{\boldsymbol{k}'} \right) \\
&= \left[+\mathrm{i} \, \partial_{\boldsymbol{k}} \Big(\frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}} u^{\alpha\tilde{a}*}_{\boldsymbol{k}} \Big) + \frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}}{\sqrt{\mathcal{N}}} \, \big(-\mathrm{i} \, \partial_{\boldsymbol{k}} u^{\alpha\tilde{a}*}_{\boldsymbol{k}} \big) \right] \left(\frac{e^{-\mathrm{i}\boldsymbol{k}'\cdot(\boldsymbol{R}-\boldsymbol{r})}}{\mathcal{N}} \, u^{\alpha\tilde{a}'}_{\boldsymbol{k}'} \right).
\end{aligned} \tag{A47}$$

To proceed, we reexpress the first term on the right-hand side as a product of two overlaps to be differentiated with respect to momentum, while we perform the implicit sum over $\boldsymbol{r} \in \Lambda_r$ on the second term on the right-hand side. This implicit sum over $\boldsymbol{r} \in \Lambda_r$ produces the multiplicative factor $\mathcal{N} \times \delta_{\boldsymbol{k},\boldsymbol{k}'}$. Thus,

$$\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \, \hat{\boldsymbol{r}} \, | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle = \left[+\mathrm{i} \, \partial_{\boldsymbol{k}} \Big(\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \psi^{\alpha}_{\boldsymbol{r}} \rangle \langle \psi^{\alpha}_{\boldsymbol{r}} | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle \Big) + \frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}} \, \big(-\mathrm{i} \, \partial_{\boldsymbol{k}} u^{\alpha\tilde{a}*}_{\boldsymbol{k}} \big) \, u^{\alpha\tilde{a}'}_{\boldsymbol{k}} \right]. \tag{A48}$$

The implicit sums over $\boldsymbol{r} \in \Lambda_r$ and $\alpha = 1, \cdots, N$ in the first term on the right-hand side delivers the resolution of the identity, while we can use the orthonormality (A6b) and (A6c) to move the momentum gradient in the second term on the right-hand side. This manipulation gives

$$\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \, \hat{\boldsymbol{r}} \, | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle = \left[+\mathrm{i} \, \partial_{\boldsymbol{k}} \Big(\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle \Big) + \frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}} \, u^{\alpha\tilde{a}*}_{\boldsymbol{k}} \, \Big(\mathrm{i} \, \partial_{\boldsymbol{k}} u^{\alpha\tilde{a}'}_{\boldsymbol{k}} \Big) \right]. \tag{A49}$$

Equations (A7) and (A17b) deliver

$$\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \, \hat{\boldsymbol{r}} \, | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle = \left[+\mathrm{i} \, \partial_{\boldsymbol{k}} \left(\frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}} \right) \, \delta^{\tilde{a},\tilde{a}'} \, + \frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}} \, \mathrm{i} \, \boldsymbol{A}^{\tilde{a}\tilde{a}'}_{\boldsymbol{k}} \right]. \tag{A50}$$

We conclude with

$$\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \, \hat{\boldsymbol{r}} \, | W^{\tilde{a}'}_{\boldsymbol{R}} \rangle = \frac{e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}}}{\sqrt{\mathcal{N}}} \, \Big(\boldsymbol{R} \, \delta^{\tilde{a},\tilde{a}'} \, + \mathrm{i} \, \boldsymbol{A}^{\tilde{a}\tilde{a}'}_{\boldsymbol{k}} \Big). \tag{A51}$$

The proof of Eq. (A42) starts from suitably modifying Eq. (A44) according to

$$\begin{aligned}
\langle \chi^{a}_{\boldsymbol{k}} | \left[\widehat{X}^{\mu}_r \, , \widehat{X}^{\nu}_r \right] \, \widehat{X}^{\lambda}_r \, | \chi^{a'}_{\boldsymbol{k}'} \rangle &= \langle \chi^{a}_{\boldsymbol{k}} | \left[|\chi^{\tilde{b}}_{\boldsymbol{p}}\rangle \, \left(-F^{\tilde{b}\tilde{b}'}_{\mu\nu;\boldsymbol{p}} \right) \, \langle \chi^{\tilde{b}'}_{\boldsymbol{p}}| \right] \, \widehat{X}^{\lambda}_r \, | \chi^{a'}_{\boldsymbol{k}'} \rangle \\
&= \delta^{a,\tilde{b}} \times \delta^{a',\tilde{a}'} \times \left(-F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}} \right) \times \langle \chi^{\tilde{b}}_{\boldsymbol{k}} | \widehat{X}^{\lambda}_r \, | \chi^{\tilde{a}'}_{\boldsymbol{k}'} \rangle
\end{aligned} \tag{A52}$$

where we can either choose the representation

$$\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \widehat{\boldsymbol{X}}_r \, | \chi^{\tilde{a}'}_{\boldsymbol{k}'} \rangle = \frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{r}}}{\mathcal{N}} \, \boldsymbol{r} \, u^{\alpha\tilde{a}*}_{\boldsymbol{k}} \, u^{\alpha\tilde{a}'}_{\boldsymbol{k}'} \tag{A53}$$

if we opt not to use the product rule for differentiation or

$$\langle \chi^{\tilde{a}}_{\boldsymbol{k}} | \widehat{\boldsymbol{X}}_r \, | \chi^{\tilde{a}'}_{\boldsymbol{k}'} \rangle = \left(\frac{e^{-\mathrm{i}(\boldsymbol{k}-\boldsymbol{k}')\cdot\boldsymbol{R}}}{\mathcal{N}} \, \boldsymbol{R} \, \delta^{\tilde{a}\tilde{a}'} + \mathrm{i} \, \boldsymbol{A}^{\tilde{a}\tilde{a}'}_{\boldsymbol{k}} \, \delta_{\boldsymbol{k},\boldsymbol{k}'} \right) \tag{A54}$$

if we opt to use the product rule for differentiation as we did in Eqs. (A22) and (A24).

□

6. Gauge invariant regularization of the trace of the 1 and 3 brackets

Equation (A40) is the main result that we need to draw a connection between the expectation value of the 3-bracket in the noninteracting filled Fermi sea and the $U(N)$ Chern-Simons action in 3-dimensional space.

We have shown in Sec. II A the "symbolic" gauge invariance of the expectation value of the 1-, 2-, and 3-bracket of the projected many-body position operator in the Fermi sea filling up $\widetilde{N}$ Bloch bands. The qualifier "symbolic" must be used since this symmetry presumes the existence of the expectation value. There is no ambiguity for the 2-bracket. The 1- and 3-brackets are however ill defined. They need to be regularized, i.e., made finite.

It is well known in quantum field theory that regularizations can break a classical symmetry. Regularizations know about quantum mechanics, for they involve expectation values of operators made of additive pieces that do not commute. In a path integral formalism, quantum mechanics is traded for coherent states at the price of a measure that requires a regularization. Here, we need to trace over an operator that can be decomposed into two additive operators that do not commute. The resulting quantum fluctuations require a regulation of ill-conditioned sums.

However, in the process of regularization the symbolic gauge invariance can disappear. The question thus becomes the following. Is it possible to regulate the 1- and 3-bracket in a gauge invariant way whereby the gauge invariance only applies to pure gauge transformation since large gauge transformations change the boundary conditions and thus the very nature of the Hilbert space over which the trace is to be performed?

Our answer is positive and relies on the observation that we already made in Eq. (A18) and follows from Eq. (A40) namely that

$$\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R = \mathrm{i}\,\widehat{\boldsymbol{A}} \tag{A55a}$$

where we have introduced the operator

$$\widehat{\boldsymbol{A}} := |\chi^{\tilde{a}}_{\boldsymbol{k}}\rangle\, \boldsymbol{A}^{\tilde{a}\tilde{b}}_{\boldsymbol{k}}\, \langle\chi^{\tilde{b}}_{\boldsymbol{k}}| \tag{A55b}$$

through its spectral decomposition.

One verifies by direct computation with the help of Eqs. (A40) and (A55) that

$$\begin{aligned} F^{(3)}_{\text{finite}}[\boldsymbol{A}] &:= \frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\widehat{X}^\mu_r\,\widehat{X}^\nu_r\,\left(\widehat{X}^\lambda_r - \widehat{X}^\lambda_R\right)\right]|W^a_{\boldsymbol{R}}\rangle \\ &= -\frac{1}{\mathcal{N}}\times\frac{\mathrm{i}}{2}\sum_{\boldsymbol{k}\in\Lambda^\star_{\text{BZ}}}\epsilon^{\mu\nu\lambda}\,F^{\tilde{a}\tilde{b}}_{\mu\nu;\boldsymbol{k}}\,A^{\tilde{b}}_{\lambda;\boldsymbol{k}} \end{aligned} \tag{A56}$$

breaks $SU(\widetilde{N})$ pure gauge symmetry. This regularization is thus not the one we seek. (Summation convention over repeated indices is implied.)

However, we immediately see that there is an ambiguity when choosing the space index for which we will do the replacement $\widehat{\boldsymbol{X}}^\mu_r \to \widehat{\boldsymbol{X}}^\mu_r - \widehat{\boldsymbol{X}}^\mu_R$. There are three possible choices that would have all lead to the same right-hand side (A56), namely

$$\begin{aligned} F^{(3)}_{\text{finite}}[\boldsymbol{A}] &= \frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\widehat{X}^\mu_r\,\widehat{X}^\nu_r\,\left(\widehat{X}^\lambda_r - \widehat{X}^\lambda_R\right)\right]|W^a_{\boldsymbol{R}}\rangle \\ &= \frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\widehat{X}^\mu_r\,\left(\widehat{X}^\nu_r - \widehat{X}^\nu_R\right)\,\widehat{X}^\lambda_r\right]|W^a_{\boldsymbol{R}}\rangle \\ &= \frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\left(\widehat{X}^\mu_r - \widehat{X}^\mu_R\right)\,\widehat{X}^\nu_r\,\widehat{X}^\lambda_r\right]|W^a_{\boldsymbol{R}}\rangle. \end{aligned} \tag{A57}$$

(Summation convention over repeated indices is implied.)

Proof. We can first insert and then remove the resolution of the identity as

$$\begin{aligned} \langle W^a_{\boldsymbol{R}}|\left[\widehat{X}^\mu_r\,\left(\widehat{X}^\nu_r - \widehat{X}^\nu_R\right)\,\widehat{X}^\lambda_r\right]|W^a_{\boldsymbol{R}}\rangle &= \langle W^a_{\boldsymbol{R}}|\widehat{X}^\mu_r\,\left(\widehat{X}^\nu_r - \widehat{X}^\nu_R\right)\,|W^{a'}_{\boldsymbol{R}'}\rangle\langle W^{a'}_{\boldsymbol{R}'}|\widehat{X}^\lambda_r\,|W^a_{\boldsymbol{R}}\rangle \\ &= \langle W^{a'}_{\boldsymbol{R}'}|\widehat{X}^\lambda_r\,|W^a_{\boldsymbol{R}}\rangle\langle W^a_{\boldsymbol{R}}|\widehat{X}^\mu_r\,\left(\widehat{X}^\nu_r - \widehat{X}^\nu_R\right)\,|W^{a'}_{\boldsymbol{R}'}\rangle \\ &= \langle W^{a'}_{\boldsymbol{R}'}|\widehat{X}^\lambda_r\,\widehat{X}^\mu_r\,\left(\widehat{X}^\nu_r - \widehat{X}^\nu_R\right)\,|W^{a'}_{\boldsymbol{R}'}\rangle \end{aligned} \tag{A58}$$

for the second line of Eq. (A57) and

$$\begin{aligned}\langle W^a_{\boldsymbol{R}}|\left[\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right)\,\widehat{X}^\nu_r\,\widehat{X}^\lambda_r\right]|W^a_{\boldsymbol{R}}\rangle&=\langle W^a_{\boldsymbol{R}}|\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right)\,|W^{a'}_{\boldsymbol{R}'}\rangle\langle W^{a'}_{\boldsymbol{R}'}|\widehat{X}^\nu_r\,\widehat{X}^\lambda_r\,|W^a_{\boldsymbol{R}}\rangle\\&=\langle W^{a'}_{\boldsymbol{R}'}|\widehat{X}^\nu_r\,\widehat{X}^\lambda_r\,|W^a_{\boldsymbol{R}}\rangle\langle W^a_{\boldsymbol{R}}|\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right)\,|W^{a'}_{\boldsymbol{R}'}\rangle\\&=\langle W^{a'}_{\boldsymbol{R}'}|\widehat{X}^\nu_r\,\widehat{X}^\lambda_r\,\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right)\,|W^{a'}_{\boldsymbol{R}'}\rangle\end{aligned}\tag{A59}$$

for the third line of Eq. (A57). The space labels $\mu,\nu,\lambda=1,\cdots,d$ have been reordered in cyclic fashion so that contraction with $\epsilon^{\mu\nu\lambda}$ delivers Eq. (A57). □

The subtraction that we performed in Eq. (A56) does regulate the expectation value of the 3-bracket but not in a gauge invariant way. Instead of Eq. (A56), we use the more symmetric definition

$$\begin{aligned}F^{(3)}_{\text{gauge invariant}}[\boldsymbol{A}]:=&+\frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\widehat{X}^\mu_r\,\widehat{X}^\nu_r\,\left(\widehat{X}^\lambda_r-\widehat{X}^\lambda_R\right)\right]|W^a_{\boldsymbol{R}}\rangle\\&+\frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\widehat{X}^\mu_r\,\left(\widehat{X}^\nu_r-\widehat{X}^\nu_R\right)\,\widehat{X}^\lambda_r\right]|W^a_{\boldsymbol{R}}\rangle\\&+\frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right)\,\widehat{X}^\nu_r\,\widehat{X}^\lambda_r\right]|W^a_{\boldsymbol{R}}\rangle\\&-\frac{1}{\mathcal{N}}\langle W^a_{\boldsymbol{R}}|\left[\epsilon_{\mu\nu\lambda}\,\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right)\,\left(\widehat{X}^\nu_r-\widehat{X}^\nu_R\right)\,\left(\widehat{X}^\lambda_r-\widehat{X}^\lambda_R\right)\right]|W^a_{\boldsymbol{R}}\rangle.\end{aligned}\tag{A60}$$

One verifies by direct computation with the help of Eqs. (A40) and (A55) that

$$F^{(3)}_{\text{gauge invariant}}[\boldsymbol{A}]=-\mathrm{i}\,\frac{3}{2}\,\frac{1}{\mathcal{N}}\sum_{\boldsymbol{k}\in\Lambda^\star_{\text{BZ}}}\epsilon^{\mu\nu\lambda}\,\mathrm{tr}\,\left(F_{\mu\nu;\boldsymbol{k}}\,A_{\lambda;\boldsymbol{k}}-\frac{2}{3}A_{\mu;\boldsymbol{k}}\,A_{\nu;\boldsymbol{k}}\,A_{\lambda;\boldsymbol{k}}\right)\tag{A61}$$

is proportional to the integral over the Brillouin zone of the Chern-Simons 3 form.

The operator over which the trace is taken on the right-hand side of Eq. (A60) can be rewritten in a way that brings it to a linear combination of 3-brackets, thereby justifying the upper index (3) for the functional $F^{(3)}_{\text{gauge invariant}}[\boldsymbol{A}]$ over the manifold of $su(\widetilde{N})$ gauge fields. Indeed, we are allowed to reorder the $3\times 6=18$ operators over which the trace is taken on the first three lines of the right-hand side of Eq. (A60) as follows,

$$\begin{aligned}\epsilon_{IJK}\left[\widehat{X}^I_r\,\widehat{X}^J_r\,\left(\widehat{X}^K_r-\widehat{X}^K_R\right)+\widehat{X}^I_r\,\left(\widehat{X}^J_r-\widehat{X}^J_R\right)\,\widehat{X}^K_r+\left(\widehat{X}^I_r-\widehat{X}^I_R\right)\,\widehat{X}^J_r\,\widehat{X}^K_r\right]=&\\\left[\widehat{X}^\mu_r,\widehat{X}^\nu_r,\left(\widehat{X}^\lambda_r-\widehat{X}^\lambda_R\right)\right]+\left[\widehat{X}^\mu_r,\left(\widehat{X}^\nu_r-\widehat{X}^\nu_R\right),\widehat{X}^\lambda_r\right]+\left[\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right),\widehat{X}^\nu_r,\widehat{X}^\lambda_r\right]&\end{aligned}\tag{A62}$$

where $I,J,K=\mu,\nu,\lambda$. One also verifies that

$$\left[\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right),\left(\widehat{X}^\nu_r-\widehat{X}^\nu_R\right),\left(\widehat{X}^\lambda_r-\widehat{X}^\lambda_R\right)\right]=\epsilon_{IJK}\,\left(\widehat{X}^I_r-\widehat{X}^I_R\right)\,\left(\widehat{X}^J_r-\widehat{X}^J_R\right)\,\left(\widehat{X}^K_r-\widehat{X}^K_R\right)\tag{A63}$$

where $I,J,K=\mu,\nu,\lambda$. We may then define the regularized 3-bracket to be the linear combination

$$\begin{aligned}\left[\widehat{X}^\mu_r,\widehat{X}^\nu_r,\widehat{X}^\lambda_r\right]_{\text{reg}}:=\frac{1}{2}\Bigg\{&\left[\widehat{X}^\mu_r,\widehat{X}^\nu_r,\left(\widehat{X}^\lambda_r-\widehat{X}^\lambda_R\right)\right]+\left[\widehat{X}^\mu_r,\left(\widehat{X}^\nu_r-\widehat{X}^\nu_R\right),\widehat{X}^\lambda_r\right]+\left[\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right),\widehat{X}^\nu_r,\widehat{X}^\lambda_r\right]\\&-\left[\left(\widehat{X}^\mu_r-\widehat{X}^\mu_R\right),\left(\widehat{X}^\nu_r-\widehat{X}^\nu_R\right),\left(\widehat{X}^\lambda_r-\widehat{X}^\lambda_R\right)\right]\Bigg\}.\end{aligned}\tag{A64}$$

Here, we have multiplied the curly braces by the normalization $1/2$ as we demand that the regularization preserves the number of 3-brackets to be regularized. To regularize a single 3-bracket, we added three 3-brackets and subtracted one 3-bracket. the number $3-1=2$ is thus the integer by which we choose to divide the curly bracket on the right-hand side of Eq. (A64). Because the regularized 3-bracket is a linear superposition of 3-brackets, it remains odd under the exchange of any pair of its consecutive arguments,

$$\left[\widehat{X}^{\sigma(\mu)}_r,\widehat{X}^{\sigma(\nu)}_r,\widehat{X}^{\sigma(\lambda)}_r\right]_{\text{reg}}=(-)^{\text{sgn}(\sigma)}\left[\widehat{X}^\mu_r,\widehat{X}^\nu_r,\widehat{X}^\lambda_r\right]_{\text{reg}}\tag{A65}$$

with σ denoting any permutation of 3 objects and $\mathrm{sgn}(\sigma) = 0, 1$ with 0 if the permutation is even and 1 if the permutation is odd. The regularized 3-bracket also vanishes whenever two of its arguments are equal,

$$\left[\widehat{X}_r^{\mu}, \widehat{X}_r^{\nu}, \widehat{X}_r^{\lambda}\right]_{\mathrm{reg}} = 0 \tag{A66}$$

if $\mu = \nu$ or $\nu = \lambda$ or $\mu = \lambda$. Finally, the regularized 3-bracket is invariant under pure gauge transformations of the form (2.39b) since

$$\left[\widehat{X}_r^{\mu}, \widehat{X}_r^{\nu}, \widehat{X}_r^{\lambda}\right]_{\mathrm{reg}} = -\mathrm{i}\,\frac{3}{4}\,\frac{1}{\mathcal{N}} \sum_{\boldsymbol{k}\in\Lambda^{\star}_{\mathrm{BZ}}} \epsilon^{IJK}\,\mathrm{tr}\,\left(F_{IJ;\boldsymbol{k}}\,A_{K;\boldsymbol{k}} - \frac{2}{3}A_{I;\boldsymbol{k}}\,A_{J;\boldsymbol{k}}\,A_{K;\boldsymbol{k}}\right) \tag{A67}$$

where $I, J, K = \mu, \nu, \lambda$.

7. Regularized 3-bracket and the Nambu bracket

We are going to prove Eq. (2.63) to which we refer the reader for the notation and definitions.

To perform a Taylor expansion on $\mathrm{Tr}\left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]_{\mathrm{reg}}$, we need to start with a Taylor expansion on

$$\begin{aligned}\left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]_{\mathrm{reg}} := &+ \left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R)\right] \\ &+ \left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R), f_3(\widehat{\boldsymbol{X}}_r)\right] \\ &+ \left[f_1(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right] \\ &- \left[f_1(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R), f_2(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R), f_3(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R)\right].\end{aligned} \tag{A68}$$

To this end, we recall that

$$[A, B, C] = A[B, C] + B[C, A] + C[A, B]. \tag{A69}$$

Thus,

$$\begin{aligned}\left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]_{\mathrm{reg}} = &+ f_1(\widehat{\boldsymbol{X}}_r)\left[f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R)\right] + \text{cyclic permutations of 1,2,3} \\ &+ f_1(\widehat{\boldsymbol{X}}_r)\left[f_2(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R), f_3(\widehat{\boldsymbol{X}}_r)\right] + \text{cyclic permutations of 1,2,3} \\ &+ f_1(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R)\left[f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right] + \text{cyclic permutations of 1,2,3} \\ &- f_1(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R)\left[f_2(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R), f_3(\widehat{\boldsymbol{X}}_r - \widehat{\boldsymbol{X}}_R)\right] - \text{cyclic permutations of 1,2,3.}\end{aligned} \tag{A70}$$

We are now ready to insert the Taylor expansions

$$f_i(\boldsymbol{x}) = f_i(\boldsymbol{0}) + \sum_{\mu=1}^{3}\left(\partial_\mu f_i\right)(\boldsymbol{0})\,x^\mu + \cdots \tag{A71}$$

for $i = 1, 2, 3$ after substituting $\boldsymbol{x}$ with the corresponding projected position operator. Because $f_i(\boldsymbol{0})$ with $i = 1, 2, 3$ are $\mathbb{C}$ numbers, the commutators in Eq. (A70) must necessarily be of second order in the projected position operators if they are to be nonvanishing. This means that the insertion of Eq. (A71) into Eq. (A70) can be organized into the expansion

$$\left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]_{\mathrm{reg}} = \left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]^{(2)}_{\mathrm{reg}} + \left[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\right]^{(3)}_{\mathrm{reg}} + \cdots \tag{A72a}$$

where

$$\begin{aligned}\Big[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\Big]^{(2)}_{\rm reg} = &+ \big[f_1\ \big(\partial_\mu f_2\big)\big(\partial_\nu f_3\big) + \text{cyclic permutations of 1,2,3}\big](\mathbf{0})\ \Big[\widehat{X}^\mu_r, \widehat{X}^\nu_r - \widehat{X}^\nu_R\Big] \\ &+ \big[f_2\ \big(\partial_\mu f_3\big)\big(\partial_\nu f_1\big) + \text{cyclic permutations of 1,2,3}\big](\mathbf{0})\ \Big[\widehat{X}^\mu_r - \widehat{X}^\mu_R, \widehat{X}^\nu_r\Big] \\ &+ \big[f_3\ \big(\partial_\mu f_1\big)\big(\partial_\nu f_2\big) + \text{cyclic permutations of 1,2,3}\big](\mathbf{0})\ \Big[\widehat{X}^\mu_r, \widehat{X}^\nu_r\Big] \\ &- \big[f_1\ \big(\partial_\mu f_2\big)\big(\partial_\nu f_3\big) + \text{cyclic permutations of 1,2,3}\big](\mathbf{0})\ \Big[\widehat{X}^\mu_r - \widehat{X}^\nu_R, \widehat{X}^\nu_r - \widehat{X}^\nu_R\Big]\end{aligned} \tag{A72b}$$

while

$$\Big[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\Big]^{(3)}_{\rm reg} = \big(\partial_\mu f_1\big)\big(\partial_\nu f_2\big)\big(\partial_\lambda f_3\big)(\mathbf{0})\ \Big[\widehat{X}^\mu_r, \widehat{X}^\nu_r, \widehat{X}^\lambda_r\Big]^{(3)}_{\rm reg}. \tag{A72c}$$

The summation convention over the repeated indices $\mu, \nu, \lambda = 1, 2, 3$ is understood. If we take advantage of the fact that

$$\Big[\widehat{X}^\mu_R, \widehat{X}^\nu_R\Big] = 0, \qquad \mu, \nu = 1, 2, 3, \tag{A73}$$

we find the remarkable simplification

$$\begin{aligned}\Big[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\Big]^{(2)}_{\rm reg} &= +2\big[f_1\ \big(\partial_\mu f_2\big)\big(\partial_\nu f_3\big) + \text{cyclic permutations of 1,2,3}\big](\mathbf{0})\ \Big[\widehat{X}^\mu_r, \widehat{X}^\nu_r\Big] \\ &= \epsilon^{ijk} f_i\ \big\{f_j, f_k\big\}^{\mu\nu}_{\rm P}(\mathbf{0})\ \Big[\widehat{X}^\mu_r, \widehat{X}^\nu_r\Big].\end{aligned} \tag{A74}$$

Another simplification due to the full antisymmetry of the 3-bracket delivers

$$\Big[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\Big]^{(3)}_{\rm reg} = \{f_1, f_2, f_3\}_{\rm N}(\mathbf{0})\ \Big[\widehat{X}^1_r, \widehat{X}^2_r, \widehat{X}^3_r\Big]_{\rm reg}. \tag{A75}$$

We thus arrive at the operator identity

$$\Big[f_1(\widehat{\boldsymbol{X}}_r), f_2(\widehat{\boldsymbol{X}}_r), f_3(\widehat{\boldsymbol{X}}_r)\Big]_{\rm reg} = \epsilon^{ijk} f_i\ \big\{f_j, f_k\big\}^{\mu\nu}_{\rm P}(\mathbf{0})\ \Big[\widehat{X}^\mu_r, \widehat{X}^\nu_r\Big] + \{f_1, f_2, f_3\}_{\rm N}(\mathbf{0})\ \Big[\widehat{X}^1_r, \widehat{X}^2_r, \widehat{X}^3_r\Big]_{\rm reg} + \cdots. \tag{A76}$$

Appendix B: Gell-Mann matrices

The Gell-Mann matrices are 3×3 Hermitian matrices that are a representation of generators of SU(3). They are defined as

$$\begin{aligned}\lambda_1 &= \begin{pmatrix}0&1&0\\1&0&0\\0&0&0\end{pmatrix}, \quad \lambda_2 = \begin{pmatrix}0&-\mathrm{i}&0\\\mathrm{i}&0&0\\0&0&0\end{pmatrix}, \quad \lambda_3 = \begin{pmatrix}1&0&0\\0&-1&0\\0&0&0\end{pmatrix}, \quad \lambda_4 = \begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}, \\ \lambda_5 &= \begin{pmatrix}0&0&-\mathrm{i}\\0&0&0\\\mathrm{i}&0&0\end{pmatrix}, \quad \lambda_6 = \begin{pmatrix}0&0&0\\0&0&1\\0&1&0\end{pmatrix}, \quad \lambda_7 = \begin{pmatrix}0&0&0\\0&0&-\mathrm{i}\\0&\mathrm{i}&0\end{pmatrix}, \quad \lambda_8 = \frac{1}{\sqrt{3}}\begin{pmatrix}1&0&0\\0&1&0\\0&0&-2\end{pmatrix}.\end{aligned} \tag{B1}$$

Appendix C: Topological invariants in the 3-orbital model

In this Appendix, we evaluate the Chern numbers

$$\mathrm{Ch}^\lambda = \frac{\mathrm{i}}{(2\pi)^2}\frac{\epsilon^{\mu\nu\lambda}}{2}\int\limits_{\rm BZ} \mathrm{d}^3\boldsymbol{k}\, F_{\mu\nu}(\boldsymbol{k}) \in \mathbb{Z}, \tag{C1}$$

for $\lambda = 1, 2, 3$ and the Chern-Simons-invariant

$$\theta := \frac{\epsilon^{\mu\nu\lambda}}{8\pi}\int\limits_{\rm BZ} \mathrm{d}^3\boldsymbol{k}\, F_{\mu\nu}(\boldsymbol{k})\, A_\lambda(\boldsymbol{k}), \tag{C2}$$

for the projection on the dispersionless middle band of the three-orbital model defined by Eq. (3.1) in the ther-

modynamic limit. (We have dropped the symbol refering to the projection for notational simplicity.) For the three-orbital model defined in Eq. (3.1), the block off-diagonal projector $q(\boldsymbol{k})$ defined in Eq. (3.5a) delivers a natural choice of gauge for the Berry connection of the flat band

$$\boldsymbol{A}(\boldsymbol{k}) = q^\dagger(\boldsymbol{k})\boldsymbol{\nabla} q(\boldsymbol{k}). \tag{C3a}$$

In this case, $\boldsymbol{A}$ can be decomposed as

$$\boldsymbol{A}(\boldsymbol{k}) = \begin{pmatrix} A'(k_1,k_2,k_3) + A''(k_1,k_2,k_3) \\ A'(k_2,k_1,k_3) - A''(k_2,k_1,k_3) \\ A_3(k_1,k_2,k_3) \end{pmatrix}, \tag{C3b}$$

where

$$A'(\boldsymbol{k}) = -\mathrm{i}\,\frac{\sin k_1 \,\sin k_3}{G(\boldsymbol{k})}, \tag{C3c}$$

$$A''(\boldsymbol{k}) = +\mathrm{i}\,\frac{\cos k_1 \,\sin k_2}{G(\boldsymbol{k})}, \tag{C3d}$$

$$A_3(\boldsymbol{k}) = -\mathrm{i}\frac{1+\cos k_3\,(\cos k_1 + \cos k_2 - M)}{G(\boldsymbol{k})}, \tag{C3e}$$

and

$$G(\boldsymbol{k}) = 3 + \left(M - \sum_{\mu=1}^{3}\cos k_\mu\right) - \sum_{\mu=1}^{3}\cos^2 k_\mu. \tag{C3f}$$

It follows that

$$\begin{aligned} A'(k_1,k_2,k_3) &= -A'(-k_1,k_2,k_3) \\ &= +A'(k_1,-k_2,k_3) \\ &= -A'(k_1,k_2,-k_3), \end{aligned} \tag{C4a}$$

as well as

$$\begin{aligned} A''(k_1,k_2,k_3) &= +A''(-k_1,k_2,k_3) \\ &= -A''(k_1,-k_2,k_3) \\ &= +A''(k_1,k_2,-k_3), \end{aligned} \tag{C4b}$$

while $A_3(\boldsymbol{k})$ is an even function of k_1, k_2, and k_3.

As a consequence, all terms appearing in $F_{13}(\boldsymbol{k})$ and $F_{23}(\boldsymbol{k})$ are an odd function of either k_1 or k_2. Thus,

$$\mathrm{Ch}^1 = \mathrm{Ch}^2 = 0. \tag{C5}$$

Furthermore,

$$\begin{aligned} \mathrm{Ch}^3 &\propto \int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, F_{12} \\ &= \int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\,\{\partial_1\,[A'(k_2,k_1,k_3) - A''(k_2,k_1,k_3)] \\ &\quad - \partial_2\,[A'(k_1,k_2,k_3) + A''(k_1,k_2,k_3)]\} \\ &= -2\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\,\partial_2 A''(k_2,k_1,k_3) \\ &= -2\,[A''(2\pi,k_1,k_3) - A''(0,k_1,k_3)] \\ &= 0, \end{aligned} \tag{C6}$$

since $\partial_2 A''(k_2,k_1,k_3)$ is a continuous function of k_2 with periodicity 2π. We conclude that the Chern numbers **Ch** defined in Eq. (C1) vanish identically.

To calculate θ defined in Eqs. (C2) we consider integrals of the form

$$\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A_\mu \partial_\nu A_\lambda, \qquad \mu \neq \nu \neq \lambda, \tag{C7}$$

which are nonvanishing in general. On one hand, defining

$$\begin{aligned} +\theta' &:= \frac{1}{8\pi}\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A_1 \partial_2 A_3 \\ &= \frac{1}{8\pi}\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A''(k_1,k_2,k_3)\partial_2 A_3(k_1,k_2,k_3), \end{aligned} \tag{C8a}$$

partial integration delivers

$$-\theta' = \frac{1}{8\pi}\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A_3 \partial_2 A_1, \tag{C8b}$$

and using the identity $A_3(k_1,k_2,k_3) = A_3(k_2,k_1,k_3)$ one obtains

$$\begin{aligned} +\theta' &= \frac{1}{8\pi}\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A_3 \partial_1 A_2, \\ -\theta' &= \frac{1}{8\pi}\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A_2 \partial_1 A_3. \end{aligned} \tag{C8c}$$

On the other hand, defining

$$+\theta'' := \frac{1}{8\pi}\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A_2 \partial_3 A_1 \tag{C8d}$$

partial integration delivers

$$-\theta'' = \frac{1}{8\pi}\int_{\mathrm{BZ}} \mathrm{d}^3\boldsymbol{k}\, A_1 \partial_3 A_2. \tag{C8e}$$

Finally, numerical evaluation of

$$\theta = 4\theta' + 2\theta'' \tag{C9}$$

reveals that θ is quantized in units of π as announced, while θ' and θ'' are not quantized and are not equal in general (see Fig. 3).

Appendix D: Equivalence of Chern-Simons and Dirac invariants

The purpose of this Appendix is to prove that the Abelian Chern-Simons invariant, defined by

$$\theta := \frac{1}{4\pi}\int_{T^3} \mathrm{d}^3\boldsymbol{k}\,\epsilon^{\mu\nu\lambda}\, A_\mu\, \partial_\nu\, A_\lambda, \tag{D1}$$

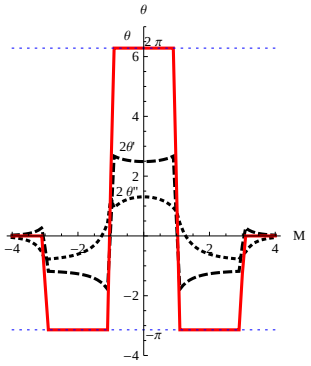

FIG. 3: (Color online) Numerical evaluation of the topological invariant $\theta^{(0)} = \pi\nu(M)$ (solid line) for the model (3.2) The parameters θ' and θ'' that sum up to the topological invariant θ are defined in Eqs. (C8a) and (C8d), respectively.

with the Abelian Berry connection $A_\mu(\boldsymbol{k})$ is equivalent to the Dirac invariant $\nu_{\rm D}$ defined in Eq. (3.10) for the case of a Bloch Hamiltonian with chiral symmetry and three bands. The topological attributes of such a Hamiltonian are characterized by its normalized off-diagonal part $q(\boldsymbol{k})$ from Eq. (3.5a) in terms of which the Abelian Berry connection reads

$$A_\mu(\boldsymbol{k}) = q^{-1}(\boldsymbol{k})\partial_\mu q(\boldsymbol{k}). \tag{D2}$$

Here, $q(\boldsymbol{k})$ represents a map from T_3 (the BZ) to S_3 and θ/π is the associated winding number. As a member of S_3, $q(\boldsymbol{k})$ can be parametrized by three angular coordinates

$$q =: \begin{pmatrix} \cos\alpha\, e^{\mathrm{i}\varphi} \\ \sin\alpha\, e^{\mathrm{i}\vartheta} \end{pmatrix}, \tag{D3}$$

and the Berry connection reads accordingly

$$A_\mu = \mathrm{i}\cos^2\alpha\,\partial_\mu\varphi + \mathrm{i}\sin^2\alpha\,\partial_\mu\vartheta, \tag{D4}$$

where we suppress the variable $\boldsymbol{k}$ for the moment. As we shall see, contributions to the winding number (D1) arise from vortex lines in $\varphi(\boldsymbol{k})$ and $\vartheta(\boldsymbol{k})$. Rewriting

$$\begin{aligned}\theta &= -\frac{\epsilon^{\mu\nu\lambda}}{4\pi}\int_{T^3} \mathrm{d}^3\boldsymbol{k}\,\sin 2\alpha\,(\partial_\mu\alpha)\,(\partial_\nu\vartheta)\,\partial_\lambda\varphi \\ &= \frac{\epsilon^{\mu\nu\lambda}}{4\pi}\Bigg\{\oint \mathrm{d}^2k_\mu\,\cos^2\alpha\,(\partial_\nu\vartheta)\,\partial_\lambda\varphi \\ &\quad - \int_{T^3}\mathrm{d}^3\boldsymbol{k}\,\cos^2\alpha\,\left[\left(\partial_\mu\partial_\nu\vartheta\right)\partial_\lambda\varphi + \left(\partial_\mu\partial_\lambda\varphi\right)\partial_\nu\vartheta\right]\Bigg\},\end{aligned} \tag{D5}$$

the antisymmetric double derivatives in the last term contribute a delta-function for $\boldsymbol{k}$ on the vortex lines times the winding of the vortex.

Let us now specialize on the model given by Eq. (3.1) in which case

$$\varphi = \arg\left(\sin k_1 + \mathrm{i}\sin k_2\right), \tag{D6}$$

$$\vartheta = \arg\left[\sin k_3 + \mathrm{i}\left(M - \sum_{i=1}^{3}\cos k_i\right)\right], \tag{D7}$$

and $\cos\alpha = 1$ in the vortex lines of φ, while $\cos\alpha = 0$ in the vortex lines of ϑ. Observe also that the first term in Eq. (D5) vanishes, since the either of the partial derivatives $\partial_\nu\vartheta$ and $\partial_\lambda\varphi$ vanishes on each surface with the normal k_μ. The four vortex lines of φ are parametrized by

$$\boldsymbol{k}^{\mathsf{T}}_{mn} := (m\pi, n\pi, k_3), \qquad m,n \in \{0,1\} \tag{D8}$$

and their winding numbers are $(-1)^{m+n}$. Eq. (D5) then simplifies to

$$\begin{aligned}\theta/\pi &= -\frac{1}{2\pi}\sum_{m,n=0}^{1}(-1)^{m+n}\int_{T^3}\mathrm{d}^3\boldsymbol{k}\,\delta(\boldsymbol{k}-\boldsymbol{k}_{mn})\partial_3\vartheta \\ &= \frac{1}{2}\sum_{m,n,l=0}^{1}(-1)^{m+n+l}\,\mathrm{sign}\,d_{\boldsymbol{k}_{mnl};4}\end{aligned} \tag{D9}$$

where we have written the number of phase windings of φ in the vortex line of ϑ as

$$\begin{aligned}-\int_0^{2\pi}\frac{\mathrm{d}k_3}{2\pi}\partial_3\vartheta(\boldsymbol{k}_{mn}) &= \frac{\mathrm{sign}\,d_{\boldsymbol{k}_{mn0};4} - \mathrm{sign}\,d_{\boldsymbol{k}_{mn1};4}}{2} \\ &= \sum_{l=0}^{1}\frac{(-1)^l}{2}\mathrm{sign}\,d_{\boldsymbol{k}_{mnl};4}\end{aligned} \tag{D10}$$

and $\boldsymbol{k}_{mnl}$ is defined as in Eq. (3.8). In writing Eq. (D9), we have recovered the Dirac invariant (3.10).

Appendix E: SMA for a flat band

We present some of the intermediate steps needed to derive Eq. (4.10a). (For ease of presentation, we use Latin instead of Greek indices for the momentum components in what follows. Summation convention over repeated indices is also implied.)

Our aim is to evaluate Eq. (4.3c) up to order $\boldsymbol{q}^2\boldsymbol{k}^2$. The commutator in Eq. (4.3c) can be conveniently broken into four contributions,

$$f_{\boldsymbol{k}} = f_{1,\boldsymbol{k}} + f_{2,\boldsymbol{k}} + f_{3,\boldsymbol{k}} + f_{4,\boldsymbol{k}}, \tag{E1a}$$

each of which read

$$f_{1,\boldsymbol{k}} := \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\left\langle\left[\delta\widehat{\rho}_{-\boldsymbol{k}}, \delta\widehat{\rho}_{-\boldsymbol{q}}\right]\left[\delta\widehat{\rho}_{+\boldsymbol{q}}, \delta\widehat{\rho}_{+\boldsymbol{k}}\right]\right\rangle, \tag{E1b}$$

$$f_{2,\boldsymbol{k}} := \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}} \left\langle \left[\delta\widehat{\rho}_{-\boldsymbol{q}}, \delta\widehat{\rho}_{+\boldsymbol{k}}\right]\left[\delta\widehat{\rho}_{-\boldsymbol{k}}, \delta\widehat{\rho}_{+\boldsymbol{q}}\right]\right\rangle, \quad \text{(E1c)}$$

$$f_{3,\boldsymbol{k}} := \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}} \left\langle \delta\widehat{\rho}_{-\boldsymbol{q}}\left[\delta\widehat{\rho}_{-\boldsymbol{k}}, \left[\delta\widehat{\rho}_{+\boldsymbol{q}}, \delta\widehat{\rho}_{+\boldsymbol{k}}\right]\right]\right\rangle, \quad \text{(E1d)}$$

and

$$f_{4,\boldsymbol{k}} := \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}} \left\langle \left[\delta\widehat{\rho}_{-\boldsymbol{k}}, \left[\delta\widehat{\rho}_{-\boldsymbol{q}}, \delta\widehat{\rho}_{+\boldsymbol{k}}\right]\right]\delta\widehat{\rho}_{+\boldsymbol{q}}\right\rangle. \quad \text{(E1e)}$$

The commutator of two projected density operators can be expressed, with the aid of Eq. (4.8), as

$$\left[\widehat{\rho}_{\boldsymbol{q}}, \widehat{\rho}_{\boldsymbol{k}}\right] = \sum_{\boldsymbol{p}} R_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}}\, \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\, \widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}+\boldsymbol{k}}, \quad \text{(E2a)}$$

where

$$R_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}} := M_{\boldsymbol{p},\boldsymbol{q}}\, M_{\boldsymbol{p}+\boldsymbol{q},\boldsymbol{k}} - M_{\boldsymbol{p}+\boldsymbol{k},\boldsymbol{q}}\, M_{\boldsymbol{p},\boldsymbol{k}}. \quad \text{(E2b)}$$

The nested commutators of three projected density operators can be expressed, with the aid of Eq. (4.8), as

$$\left[\widehat{\rho}_{\boldsymbol{k}}, \left[\widehat{\rho}_{\boldsymbol{q}}, \widehat{\rho}_{\boldsymbol{k}}\right]\right] = \sum_{\boldsymbol{p}} \Lambda_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}}\, \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\, \widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}}, \quad \text{(E3a)}$$

where

$$\Lambda_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}} := R_{\boldsymbol{p}-\boldsymbol{k},\boldsymbol{q},\boldsymbol{k}}\, M_{\boldsymbol{p},-\boldsymbol{k}} - R_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}}\, M_{\boldsymbol{p}+\boldsymbol{q}+\boldsymbol{k},-\boldsymbol{k}}. \quad \text{(E3b)}$$

Observe here that the identity

$$\left[\widehat{\rho}_{\boldsymbol{k}}, \left[\widehat{\rho}_{\boldsymbol{q}}, \widehat{\rho}_{\boldsymbol{k}}\right]\right]^{\dagger} = \left[\widehat{\rho}_{-\boldsymbol{k}}, \left[\widehat{\rho}_{-\boldsymbol{q}}, \widehat{\rho}_{-\boldsymbol{k}}\right]\right] \quad \text{(E4)}$$

implies that

$$\Lambda^{*}_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}} = \Lambda_{\boldsymbol{p}+\boldsymbol{q},-\boldsymbol{q},-\boldsymbol{k}}. \quad \text{(E5)}$$

Needed is the expansion of $R_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}}$ and $\Lambda_{\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}}$ up to order $\boldsymbol{q}^2\boldsymbol{k}^2$. We start with

$$\begin{aligned} M_{\boldsymbol{p},\boldsymbol{q}} &= u^{\dagger}_{\boldsymbol{p}} \cdot u_{\boldsymbol{p}+\boldsymbol{q}} \\ &= u^{\dagger}_{\boldsymbol{p}} \cdot \left(u_{\boldsymbol{p}} + q^i\, \partial_i u_{\boldsymbol{p}} + \frac{1}{2}\, q^i q^j\, \partial_i \partial_j u_{\boldsymbol{p}} + \cdots\right) \\ &= 1 + q^i\, u^{\dagger}_{\boldsymbol{p}} \cdot \partial_i u_{\boldsymbol{p}} + \frac{1}{2}\, q^i q^j\, u^{\dagger}_{\boldsymbol{p}} \cdot \partial_i \partial_j u_{\boldsymbol{p}} + \cdots \\ &= 1 + q^i\, A_{i,\boldsymbol{p}} + \frac{1}{2}\, q^i q^j\, u^{\dagger}_{\boldsymbol{p}} \cdot \partial_i \partial_j u_{\boldsymbol{p}} + \cdots \end{aligned} \quad \text{(E6a)}$$

where we have introduced the (imaginary-valued) Berry connection

$$A_{i,\boldsymbol{p}} \equiv u^{\dagger}_{\boldsymbol{p}} \cdot \partial_i u_{\boldsymbol{p}} \quad \text{(E6b)}$$

and the summation convention over repeated indices $i, j = 1, \cdots, d$ is implied. The symbol ∂_i with $i = 1, \cdots, d$ is to be regarded as a derivative with respect to the argument of the function on which it acts. Similarly,

$$\begin{aligned} M_{\boldsymbol{p}+\boldsymbol{q},\boldsymbol{k}} = 1 &+ k^i\, A_i + q^i k^j \partial_i u^{\dagger} \cdot \partial_j u + \frac{1}{2}\left(k^i k^j + 2 q^i k^j\right)\, u^{\dagger} \cdot \partial_i \partial_j u \\ &+ \frac{1}{2}\left(q^i q^j k^m + k^i k^j q^m\right)\, u^{\dagger} \cdot \partial_i \partial_j \partial_m u + \frac{1}{2}\left(k^i k^j q^m + 2 q^m q^i k^j\right)\, \partial_m u^{\dagger} \cdot \partial_i \partial_j \partial_m u + \frac{1}{2}\, q^i q^j k^m\, \partial_i \partial_j u^{\dagger} \cdot \partial_m u \\ &+ \frac{1}{4}\, q^i q^j k^l k^m\, u^{\dagger} \cdot \partial_i \partial_j \partial_l \partial_m u + \frac{1}{2}\, k^i k^j q^l q^m\, \partial_l u^{\dagger} \cdot \partial_i \partial_j \partial_m u + \frac{1}{2}\, q^i q^j k^l k^m\, \partial_i \partial_j u^{\dagger} \cdot \partial_l \partial_m \partial_m u + \cdots \end{aligned} \quad \text{(E7)}$$

where the summation convention over the repeated indices $i, j, l, m = 1, \cdots, d$ is implied.

We multiply Eq. (E6a) by Eq. (E7) and antisymmetrize with respect to the interchange of $\boldsymbol{q}$ and $\boldsymbol{k}$. We obtain

$$R(\boldsymbol{p}, \boldsymbol{q}, \boldsymbol{k}) = q^i k^j \left(T^{(2)}_{ij}\right)(\boldsymbol{p}) + \left(k^i k^j q^m - q^i q^j k^m\right)\left(T^{(3)}_{ij;m}\right)(\boldsymbol{p}) + k^i k^j q^l q^m \left(T^{(4)}_{ij;lm}\right)(\boldsymbol{p}), \quad \text{(E8a)}$$

where the summation convention over the repeated indices $i, j, l, m = 1, \cdots, d$ is implied and we have introduced the short-hand notation

$$\left(T^{(2)}_{ij}\right)(\boldsymbol{p}) := \left(F_{ij}\right)(\boldsymbol{p}) \equiv \left(\partial_i A_j - \partial_i A_j\right)(\boldsymbol{p}), \quad \text{(E8b)}$$

$$\left(T^{(3)}_{ij;m}\right)(\boldsymbol{p}) := \frac{1}{2}\left(\partial_m u^\dagger\cdot\partial_i\partial_j u - \partial_i\partial_j u^\dagger\cdot\partial_m u - 2\partial_j u^\dagger\cdot\partial_i\partial_m u - 2A_j\partial_i A_m\right)(\boldsymbol{p}), \tag{E8c}$$

and

$$\begin{aligned}\left(T^{(4)}_{ij;lm}\right)(\boldsymbol{p}) := \frac{1}{4}\Big[&\partial_l\partial_m u^\dagger\cdot\partial_i\partial_j u - \partial_i\partial_j u^\dagger\cdot\partial_l\partial_m u + 2A_l\partial_m\left(u^\dagger\cdot\partial_i\partial_j u\right) - 2A_i\partial_j\left(u^\dagger\cdot\partial_l\partial_m u\right)\\ &+ 2\partial_l u^\dagger\cdot\partial_i\partial_j\partial_m u - 2\partial_i u^\dagger\cdot\partial_l\partial_j\partial_m u\Big](\boldsymbol{p})\end{aligned} \tag{E8d}$$

for $i,j,l,m = 1,\cdots,d$. We evaluate

$$\begin{aligned}\Lambda(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) &= R(\boldsymbol{p}-\boldsymbol{k},\boldsymbol{q},\boldsymbol{k})\,M(\boldsymbol{p},-\boldsymbol{k}) - R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k})\,M(\boldsymbol{p}+\boldsymbol{q}+\boldsymbol{k},-\boldsymbol{k})\\
&= \Big[R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) - k^a\partial_a R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) + \cdots\Big]\Big[1 - k^b A_b(\boldsymbol{p}) + \cdots\Big] - R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k})\Big[1 - k^a A_a(\boldsymbol{p}) - k^a q^b\partial_b A_a(\boldsymbol{p}) + \cdots\Big]\\
&= R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) - k^a\partial_a R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) - k^a A_a(\boldsymbol{p})R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) + \cdots\\
&\quad - R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) + k^a A_a(\boldsymbol{p})R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) + k^a q^b\partial_b A_a(\boldsymbol{p})R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) + \cdots\\
&= -k^a\partial_a R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) + k^a q^b\partial_b A_a(\boldsymbol{p})R(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k}) + \cdots\\
&= -k^a\Big[q^i k^j\left(\partial_a T^{(2)}_{ij}\right)(\boldsymbol{p}) + -q^i q^j k^m\left(\partial_a T^{(3)}_{ij;m}\right)(\boldsymbol{p}) + \cdots\Big] + k^a q^b\partial_b A_a(\boldsymbol{p})\Big[q^i k^j\left(T^{(2)}_{ij}\right)(\boldsymbol{p}) + \cdots\Big]\\
&= -q^i k^j k^a\left(\partial_a T^{(2)}_{ij}\right)(\boldsymbol{p}) + q^i q^j k^m k^a\left(\partial_a T^{(3)}_{ij;m}\right)(\boldsymbol{p}) + q^b k^a q^i k^j\partial_b A_a(\boldsymbol{p})\left(T^{(2)}_{ij}\right)(\boldsymbol{p}) + \cdots\end{aligned} \tag{E9}$$

where the summation convention over the repeated indices $a,b,i,j,m = 1,\cdots,d$ is implied.

At last, we are in a position to evaluate the terms contributing to the function $f_{\boldsymbol{k}}$ in Eq. (E1). We start with

$$\begin{aligned}f_{1,\boldsymbol{k}} &= \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\left\langle[\delta\widehat{\rho}_{-\boldsymbol{k}},\delta\widehat{\rho}_{-\boldsymbol{q}}][\delta\widehat{\rho}_{\boldsymbol{q}},\delta\widehat{\rho}_{\boldsymbol{k}}]\right\rangle\\
&= \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\left\langle\sum_{\boldsymbol{p}} R(\boldsymbol{p},-\boldsymbol{k},-\boldsymbol{q})\,\widehat{\chi}^\dagger_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\sum_{\boldsymbol{p}'} R(\boldsymbol{p}',\boldsymbol{q},\boldsymbol{k})\,\widehat{\chi}^\dagger_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\right\rangle\\
&= \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} R(\boldsymbol{p},-\boldsymbol{k},-\boldsymbol{q})\,R(\boldsymbol{p}',\boldsymbol{q},\boldsymbol{k})\left\langle\widehat{\chi}^\dagger_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^\dagger_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\right\rangle\\
&= \frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[(-k^a)(-q^b)\left(T^{(2)}_{ab}\right)(\boldsymbol{p}) + \cdots\Big]\Big[q^i k^j\left(T^{(2)}_{ij}\right)(\boldsymbol{p}') + \cdots\Big]\left\langle\widehat{\chi}^\dagger_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^\dagger_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\right\rangle\\
&= -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[k^a q^b\left(F_{ab}\right)(\boldsymbol{p})\Big]\Big[k^i q^j\left(F_{ij}\right)(\boldsymbol{p}')\Big]\left\langle\widehat{\chi}^\dagger_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^\dagger_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\right\rangle + \cdots\\
&= -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\boldsymbol{B}(\boldsymbol{p})\Big]\Big[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\boldsymbol{B}(\boldsymbol{p}')\Big]\left\langle\widehat{\chi}^\dagger_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^\dagger_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\right\rangle + \cdots,\end{aligned} \tag{E10}$$

where we used that $B^i = \epsilon^{ijm}\partial_j A_m = \frac{1}{2}\epsilon^{ijm}F_{jm}$ or, equivalently, $F_{ij} = \epsilon_{ijm}B^m$. We now break the Berry field

strength into two contributions, i.e., $\boldsymbol{B}(\boldsymbol{p}) = \overline{\boldsymbol{B}} + \delta\boldsymbol{B}(\boldsymbol{p})$. If so,

$$
\begin{aligned}
f_{1,\boldsymbol{k}} &= -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\big(\overline{\boldsymbol{B}}+\delta\boldsymbol{B}(\boldsymbol{p})\big)\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\big(\overline{\boldsymbol{B}}+\delta\boldsymbol{B}(\boldsymbol{p}')\big)\,\Big]\Big\langle \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\Big\rangle + \cdots \\
&= -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big\langle \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\Big\rangle \\
&\quad -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p}')\,\Big]\Big\langle \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\Big\rangle \\
&\quad -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p})\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big\langle \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\Big\rangle \\
&\quad -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p})\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p}')\,\Big]\Big\langle \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\Big\rangle + \cdots \\
&= -\frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big\langle \widehat{\rho}_{-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\rho}_{\boldsymbol{k}+\boldsymbol{q}}\Big\rangle \\
&\quad -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p}')\,\Big]\Big\langle \widehat{\rho}_{-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\Big\rangle \\
&\quad -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p})\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\overline{\boldsymbol{B}}\,\Big]\Big\langle \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\rho}_{\boldsymbol{k}+\boldsymbol{q}}\Big\rangle \\
&\quad -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p})\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p}')\,\Big]\Big\langle \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}-\boldsymbol{k}-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}'}\,\widehat{\chi}_{\boldsymbol{p}'+\boldsymbol{k}+\boldsymbol{q}}\Big\rangle + \cdots\,.
\end{aligned}
\tag{E11}
$$

In a uniform liquid-like ground state we have $\langle\,\widehat{\rho}_{\boldsymbol{k}}\,\rangle \propto \delta_{\boldsymbol{k},\boldsymbol{0}}$ and, due to the relation $k^a q^b\, F_{ab} = (\boldsymbol{k}\wedge\boldsymbol{q})\cdot\boldsymbol{B}$, we can replace $\widehat{\rho}_{\pm\boldsymbol{k}\pm\boldsymbol{q}}$ by $\delta\widehat{\rho}_{\pm\boldsymbol{k}\pm\boldsymbol{q}}$. As a consequence, we can drop the first three terms on the last equality of (E11) up to order $\boldsymbol{q}^2\boldsymbol{k}^2$. We are then left with:

$$
f_{1,\boldsymbol{k}} = -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p})\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p}')\,\Big]\Big\langle \hat{n}_{\boldsymbol{p}}\hat{n}_{\boldsymbol{p}'}\Big\rangle + \cdots\,,
\tag{E12}
$$

where $\hat{n}_{\boldsymbol{p}} \equiv \widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}}$ is the number operator projected on the lowest band. Similarly,

$$
\begin{aligned}
f_{2,\boldsymbol{k}} &= \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\Big\langle [\delta\widehat{\rho}_{-\boldsymbol{q}},\delta\widehat{\rho}_{\boldsymbol{k}}][\delta\widehat{\rho}_{-\boldsymbol{k}},\delta\widehat{\rho}_{\boldsymbol{q}}]\Big\rangle \\
&= \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\Big\langle [\delta\widehat{\rho}_{\boldsymbol{k}},\delta\widehat{\rho}_{-\boldsymbol{q}}][\delta\widehat{\rho}_{\boldsymbol{q}},\delta\widehat{\rho}_{-\boldsymbol{k}}]\Big\rangle \\
&= f_{1,-\boldsymbol{k}} \\
&= -\frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p})\,\Big]\Big[\,(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p}')\,\Big]\Big\langle \hat{n}_{\boldsymbol{p}}\hat{n}_{\boldsymbol{p}'}\Big\rangle + \cdots\,,
\end{aligned}
\tag{E13}
$$

while

$$
\begin{aligned}
f_{3,\boldsymbol{k}} &= \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\Big\langle\, \delta\widehat{\rho}_{-\boldsymbol{q}}\,[\delta\widehat{\rho}_{-\boldsymbol{k}},\,[\delta\widehat{\rho}_{\boldsymbol{q}},\delta\widehat{\rho}_{\boldsymbol{k}}]\,]\Big\rangle \\
&= \frac{1}{2}\sum_{\boldsymbol{q}} v_{\boldsymbol{q}}\Big\langle\, \delta\widehat{\rho}_{-\boldsymbol{q}}\sum_{\boldsymbol{p}}\Lambda(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k})\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}}\Big\rangle \\
&= \frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p}} v_{\boldsymbol{q}}\,\Lambda(\boldsymbol{p},\boldsymbol{q},\boldsymbol{k})\Big\langle\, \delta\widehat{\rho}_{-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}}\Big\rangle.
\end{aligned}
\tag{E14}
$$

The matrix element $\Big\langle\, \delta\widehat{\rho}_{-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}}\Big\rangle$ vanishes in the limit $\boldsymbol{q}\to 0$ and, therefore, the only term that contributes to

$f_{3,\boldsymbol{k}}$ up to order $\boldsymbol{q}^2\boldsymbol{k}^2$ is

$$\begin{aligned} f_{3,\boldsymbol{k}} &= \frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p}} v_{\boldsymbol{q}}\Big[-q^i k^j k^a\left(\partial_a F_{ij}\right)(\boldsymbol{p})\Big]\Big\langle\,\delta\widehat{\rho}_{-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}}\Big\rangle \\ &= \frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p}} v_{\boldsymbol{q}}\Big[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\left(\frac{\partial\boldsymbol{B}}{\partial p^a}\right)(\boldsymbol{p})\Big]k^a\Big\langle\,\delta\widehat{\rho}_{-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}}\Big\rangle. \end{aligned} \tag{E15}$$

The condition (E5) implies that $f_{4,\boldsymbol{k}} = f^{*}_{3,\boldsymbol{k}}$, which then delivers

$$f_{4,\boldsymbol{k}} = \frac{1}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p}} v_{\boldsymbol{q}}\Big[-(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\left(\frac{\partial\boldsymbol{B}}{\partial p^a}\right)(\boldsymbol{p})\Big]k^a\Big\langle\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}+\boldsymbol{q}}\,\widehat{\chi}_{\boldsymbol{p}}\delta\widehat{\rho}_{\boldsymbol{q}}\,\Big\rangle, \tag{E16}$$

where we have used that $(\boldsymbol{B}(\boldsymbol{p}))^{*} = -\boldsymbol{B}(\boldsymbol{p})$.

Putting together all the contributions, we obtain

$$\begin{aligned} f_{\boldsymbol{k}} = &-\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p},\boldsymbol{p}'} v_{\boldsymbol{q}}\Big[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p})\Big]\Big[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\delta\boldsymbol{B}(\boldsymbol{p}')\Big]\Big\langle\hat{n}_{\boldsymbol{p}}\hat{n}_{\boldsymbol{p}'}\Big\rangle \\ &+\frac{k^a}{2}\sum_{\boldsymbol{q}}\sum_{\boldsymbol{p}} v_{\boldsymbol{q}}\left[(\boldsymbol{k}\wedge\boldsymbol{q})\cdot\left(\frac{\partial\boldsymbol{B}}{\partial p^a}\right)(\boldsymbol{p})\,\big\langle\delta\widehat{\rho}_{-\boldsymbol{q}}\,\widehat{\chi}^{\dagger}_{\boldsymbol{p}}\,\widehat{\chi}_{\boldsymbol{p}+\boldsymbol{q}}\big\rangle - (\boldsymbol{k}\wedge\boldsymbol{q})\cdot\left(\frac{\partial\boldsymbol{B}}{\partial p^a}\right)(\boldsymbol{p})\Big\langle\widehat{\chi}^{\dagger}_{\boldsymbol{p}+\boldsymbol{q}}\,\widehat{\chi}_{\boldsymbol{p}}\,\delta\widehat{\rho}_{\boldsymbol{q}}\,\Big\rangle\right] \end{aligned} \tag{E17}$$

where the summation convention over the repeated indices $a = 1, \cdots, d$ is implied. Finally, the analytical continuation $\boldsymbol{\mathcal{B}} \equiv -\mathrm{i}\boldsymbol{B}$ delivers Eq. (4.10a).

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