

Gauge-invariant projector calculus for quantum state geometry and applications to observables in crystals

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(Received 5 December 2024; accepted 25 June 2025; published 5 August 2025)

The importance of simple geometrical invariants, such as the Berry curvature and quantum metric, constructed from the Bloch states of a crystal has become well established over four decades of research. More complex aspects of geometry emerge in properties linking multiple bands, such as optical responses. In the companion work [Phys. Rev. Lett. **135**, 066901 (2025)], we introduced multistate geometrical invariants using an explicitly gauge-invariant formalism based on projection operators, which we used to clarify the relation between the shift current and the theory of electronic polarization among other advancements for second-order nonlinear optics. Here, we provide considerably more detail on the projector formalism and the geometrical invariants arising in the vicinity of a specific value of crystal momentum. We combine the introduction to multistate quantum geometry with broadly relevant algebraic relationships and detailed example calculations, enabling extensions toward future applications to topological and geometrical properties of insulators and metals.

DOI: [10.1103/qscv-qxqt](https://doi.org/10.1103/qscv-qxqt)

I. INTRODUCTION

The integer quantum Hall effect and topological insulators can be understood as arising from topological invariants of Bloch states in crystals. The work of Thouless and collaborators to understand the Hall effect [1] led eventually to an appreciation that the same geometrical objects that appear as integrands in topological invariants can also have physical implications of their own, including at a single point in momentum space. For example, the Berry curvature that integrates to the Chern number also determines, at each momentum point, the anomalous velocity in the semiclassical equations of motion for a Bloch wave packet [2–4]. A practical advantage in expressing the Berry curvature, particularly when its derivatives need to be evaluated, or it needs to be integrated globally, came from the realization that it can be expressed in a gauge-invariant form using projection operators [5].

The two most studied geometrical invariants of this type are the quantum metric and Berry curvature, which can be understood as the real and imaginary parts of a single quantum geometric tensor [6]. The presented work is motivated by the realization that, even at a single point in momentum space,

further geometrical objects emerge considering physical properties linking multiple bands, and that this *multistate geometry* can be expressed and computed efficiently using projection operators. The physical consequences of that observation for shift currents and polarization, including calculations for some materials of current interest, are the focus of a short companion article; see Ref. [7]. In particular, we systematically developed the theory of these geometrical objects and explained how they characterize aspects of the Bloch states that go beyond the quantum metric and Berry curvature. In the following, we provide a detailed introduction to local single- and multistate geometric invariants in combination with valuable identities and step-by-step examples, enabling the application of geometric concepts within the projector formalism to further observables in crystals.

As in classic works on the Berry curvature [5] and successfully applied in a broad class of applications [8–14], the basic idea of using projectors built from Bloch states instead of the Bloch states themselves is to avoid the ambiguous momentum-dependent phase. Avoiding this gauge dependence not only simplifies standard perturbation-theoretical approaches using Green’s function methods [15] and allows for their efficient computation, as we will discuss in the context of nonlinear optical responses, but allows for a geometrical interpretation of the complex projective bundle that the Bloch states form over the Brillouin zone. The core of this approach is using differential geometry to establish relationships among projector objects, identifying a small set of independent geometric invariants and inequalities that underpin observable relationships. In many circumstances, observables can be expressed as scalar quantities (e.g., trace or determinant) derived from projectors, which suggest a

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TABLE I. We present all geometric invariants introduced and discussed throughout this paper in their projector form.

	Single state	Two state
Quantum geometric tensor	$Q_{\alpha\beta} = \text{tr}[\hat{P} \partial_\alpha \hat{P} \partial_\beta \hat{P}]$	$Q_{\alpha\beta}^{mn} = \text{tr}[\hat{P}_n \partial_\alpha \hat{P}_m \partial_\beta \hat{P}_n]$
Quantum geometric connection	$Q_{\alpha;\beta\gamma} = \text{tr}[\hat{P} \partial_\alpha \hat{P} \partial_\beta \partial_\gamma \hat{P}]$	$C_{\alpha;\beta\gamma}^{mn} = \text{tr}[\hat{P}_n \partial_\alpha \hat{P}_m (\partial_\beta \partial_\gamma \hat{P}_n + \partial_\alpha \hat{P}_m \partial_\gamma \hat{P}_n)]$
Quantum metric	$g_{\alpha\beta} = \frac{1}{2} \text{tr}[\partial_\alpha \hat{P} \partial_\beta \hat{P}]$	$g_{\alpha\beta}^{mn} = \frac{1}{2} \text{tr}[\partial_\alpha \hat{P}_m \partial_\beta \hat{P}_n]$
Berry curvature	$\Omega_{\alpha\beta} = i \text{tr}[\hat{P} \partial_\alpha \hat{P} \partial_\beta \hat{P}] - (\alpha \leftrightarrow \beta)$	$\Omega_{\alpha\beta}^{mn} = i \text{tr}[\hat{P}_n \partial_\alpha \hat{P}_m \partial_\beta \hat{P}_n] - (\alpha \leftrightarrow \beta)$
Quantum metric dipole	$\partial_\alpha g_{\beta\gamma} = \frac{1}{2} \text{tr}[\partial_\beta \hat{P} \partial_\alpha \partial_\gamma \hat{P}] + (\beta \leftrightarrow \gamma)$	$\partial_\alpha g_{\beta\gamma}^{mn} = \frac{1}{2} \text{tr}[\partial_\alpha (\partial_\beta \hat{P}_m \partial_\gamma \hat{P}_n)]$
Berry curvature dipole	$\partial_\alpha \Omega_{\beta\gamma} = i \text{tr}[(\hat{P} \partial_\beta \hat{P} - \partial_\beta \hat{P} \hat{P}) \partial_\alpha \partial_\gamma \hat{P}] - (\beta \leftrightarrow \gamma)$	$\partial_\alpha \Omega_{\beta\gamma}^{mn} = i \text{tr}[\partial_\alpha (\hat{P}_n \partial_\beta \hat{P}_m \partial_\gamma \hat{P}_n)] - (\beta \leftrightarrow \gamma)$
Skewness tensor	$\text{Im } Q_{(\alpha;\beta\gamma)} = \frac{1}{3} \text{Im}[Q_{\alpha;\beta\gamma} + Q_{\beta;\gamma\alpha} + Q_{\gamma;\alpha\beta}]$	
Torsion tensor		$T_{\beta;\alpha\gamma}^{mn} = \text{tr}[\hat{P}_n \partial_\beta \hat{P}_m \partial_\alpha \hat{P}_m \partial_\gamma \hat{P}_n] - (\alpha \leftrightarrow \gamma)$
Shift vector		$R_{\alpha\beta}^{mn}(\mathbf{k}) = i C_{\alpha;\beta\beta}^{mn}(\mathbf{k}) / Q_{\beta\beta}^{mn}(\mathbf{k})$

geometrical form that illuminates physical content beyond topological invariants. Conversely, any such scalar is, in principle, observable, providing pathways toward unexplored observables and their physical phenomenology. This work focuses on a universal geometric approach to quantum states based on projectors arising from a Bloch Hamiltonian of a noninteracting multiorbital lattice system. Here, orthogonal, possibly degenerate, projectors parametrized by quasimomentum complement the information yielded by the energy bands. We explicitly demonstrate that geometric invariants arise in several examples, which capture quantum state properties beyond the quantum geometric tensor and objects that reduce to it, such as the quantum metric dipole, Berry curvature dipole, and Riemannian tensors. Identifying and physically interpreting geometric invariants is a subject of ongoing work [11–14, 16–32].

The paper is structured as follows. In Sec. II, we introduce the basic concepts and quantities for quantum state geometry and projector calculus. After presenting the recently emerging terminology for quantum state geometry beyond the quantum geometric tensor in Secs. II A to II E, we summarize the main geometric invariants that are currently intensively studied in Sec. II F; see an overview of these quantities in projector form in Table I. We close by various valuable projector identities for applying the projector formalism in the derivations of observables in Sec. II G. We demonstrate the formalism in two applications in Sec. III, demonstrating the close connection to the modern theory of polarization in Sec. III A and exemplifying the derivation of a nonlinear response function via a detailed derivation of the injection and shift current in Sec. III B. We provide the main conclusion and a short outlook in Sec. IV. Further technical details are given in the Appendixes.

II. PROJECTOR CALCULUS FOR QUANTUM STATE GEOMETRY

We introduce the essential techniques of projector calculus for quantum state geometry, focusing on the aspects that enable a profound understanding of the applications on the polarization distribution and shift current presented in the short companion article [7] and guide future applications to other observables in crystals. For simplicity and concreteness, we restrict ourselves to noninteracting Bloch Hamiltonians and

leave a comprehensive description of quantum state geometry in the context of interacting multiorbital lattice systems for future work. For a first introduction in this direction, we refer to Ref. [14], which revealed the Berry curvature variance and further barely-explored geometric invariants in the context of the Drude weight of interacting flatband systems.

In the following, we introduce the projectors for nondegenerate and degenerate bands, enabling us to express scalar observables in the context of quantum state geometry. We report on recent progress in identifying the minimal quantum geometric structures and we provide a summary of geometric invariants of current interest; see Table I. We conclude this section with useful projector identities that simplify the subsequent applications.

A. Projectors for nondegenerate bands

We start with a Bloch Hamiltonian $\hat{H}(\mathbf{k})$ involving N bands as a function of lattice momentum $\mathbf{k}$ in d dimensions. When diagonalized for a fixed momentum, we obtain the eigenvalues $E_n(\mathbf{k})$ and corresponding orthonormal eigenvectors $|u_n(\mathbf{k})\rangle$ with band index n . In the case of only nondegenerate bands, we construct the band projectors $\hat{P}_n(\mathbf{k})$ as the tensor product between the eigenvectors $|u_n(\mathbf{k})\rangle$ and its conjugate transpose $\langle u_n(\mathbf{k})|$, resulting in

$$\hat{P}_n(\mathbf{k}) = |u_n(\mathbf{k})\rangle \langle u_n(\mathbf{k})|. \quad (1)$$

No specific $U(1)$ gauge choice is required for $|u_n(\mathbf{k})\rangle$ within this construction as long as $\langle u_n(\mathbf{k})|$ is obtained from the corresponding $|u_n(\mathbf{k})\rangle$ since

$$\hat{P}_n(\mathbf{k}) \rightarrow e^{i\phi_n(\mathbf{k})} \hat{P}_n(\mathbf{k}) e^{-i\phi_n(\mathbf{k})} = \hat{P}_n(\mathbf{k}). \quad (2)$$

The gauge-invariant projector calculus harnesses the following four main properties. The projectors are Hermitian, idempotent, and orthogonal; that is, they satisfy

$$(\hat{P}_n(\mathbf{k}))^\dagger = \hat{P}_n(\mathbf{k}) \quad (3)$$

and

$$\hat{P}_n(\mathbf{k}) \hat{P}_m(\mathbf{k}) = \delta_{nm} \hat{P}_m(\mathbf{k}), \quad (4)$$

where the product of two projectors is defined as ordinary matrix multiplication and δ_{nm} is the Kronecker delta. As the projectors are defined with respect to the eigenstates of a given

Bloch Hamiltonian $\hat{H}(\mathbf{k})$, they further satisfy

$$\hat{H}(\mathbf{k}) \hat{P}_n(\mathbf{k}) = E_n(\mathbf{k}) \hat{P}_n(\mathbf{k}) \quad (5)$$

and

$$\sum_n \hat{P}_n(\mathbf{k}) = \mathbb{1}_N, \quad (6)$$

under summation over all N bands. Traces over products of projectors are understood as traces of the respective matrix. For instance, the Bloch-state overlap at different momenta and bands in projector form reads

$$\text{tr}[\hat{P}_n(\mathbf{k}) \hat{P}_m(\mathbf{k}')] = |\langle u_n(\mathbf{k}) | u_m(\mathbf{k}') \rangle|^2. \quad (7)$$

A key advantage in working with projectors instead of Bloch wave functions is the possibility of an efficient analytical and numerical evaluation of *geometric invariants*, that is, combinations of multiple projectors and their derivatives at the same or different momenta. The main reason for this efficiency is the elimination of gauge ambiguity of the band basis. In particular, derivatives of projectors, formally defined as

$$\partial_\alpha \hat{P}_n(\mathbf{k}) \equiv \lim_{\delta \rightarrow 0} \frac{1}{\delta} [\hat{P}_n(\mathbf{k} + \delta \mathbf{e}_\alpha) - \hat{P}_n(\mathbf{k})], \quad (8)$$

with the short notation of the derivative $\partial_\alpha \equiv \partial / \partial k_\alpha$ in direction $\mathbf{e}_\alpha$, are well defined and straightforwardly numerically implemented; see Appendix A.

Closed analytic forms of the projector in terms of the Bloch Hamiltonian without the need of any diagonalization are particularly useful. The projectors onto the lower and upper band of a two band system expressed in the form $\hat{H}(\mathbf{k}) = d_0(\mathbf{k}) + \mathbf{d}(\mathbf{k}) \cdot \boldsymbol{\sigma}$ with Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ serve as an important example and read

$$\hat{P}_\pm(\mathbf{k}) = \frac{1}{2} \left[\mathbb{1}_2 \pm \frac{\mathbf{d}(\mathbf{k})}{|\mathbf{d}(\mathbf{k})|} \cdot \boldsymbol{\sigma} \right]. \quad (9)$$

Recently, a growing number of results are available that offer closed analytic formulas for projectors directly obtained in terms of the Hamiltonian for more than two bands without any explicit diagonalization of the Hamiltonian [8,9], which we discuss in more detail in Appendix B. Expressing geometric invariants via derivatives of the Bloch Hamiltonian itself is possible for special cases, such as the Berry curvature [33], via the identities introduced in Sec. II G.

B. Projectors for degenerate bands and larger subsets

The projector formalism naturally includes the case of degenerate bands and, thus, offers their theoretical description on an equal footing. If the band is formed by $|u_{ns}(\mathbf{k})\rangle$ with $s = 1, \dots, M$ indexing the states within the M -fold degenerate band (we assume degeneracy at all $\mathbf{k}$), the projector on the degenerate subspace reads

$$\hat{P}_n(\mathbf{k}) = \sum_{s=1}^M |u_{ns}(\mathbf{k})\rangle \langle u_{ns}(\mathbf{k})|. \quad (10)$$

The same basic properties (3) to (6) hold. These projectors explicitly respect the required $U(M)$ gauge invariance of the degenerate band. In addition, it might be convenient to combine multiple bands n_1 to n_M into one subspace of quantum

states of interest,

$$\hat{P}_{(n_1 \dots n_M)}(\mathbf{k}) = \sum_{i=1}^M \hat{P}_{n_i}(\mathbf{k}), \quad (11)$$

which still satisfy the projector properties (3) and (4). The most common example is the projector onto occupied states, which takes the form $\hat{P}_{\text{occ}}(\mathbf{k}) = \sum_{n \in \text{occ}} \hat{P}_n(\mathbf{k})$.

C. Global and local geometric invariants

Being gauge invariant and Hermitian, projectors are, in principle, measurable and, thus, offer minimal building blocks to construct observables. The projectors $\hat{P}(\mathbf{k})$ constructed from a given Bloch Hamiltonian $\hat{H}(\mathbf{k})$ capture the nontrivial momentum dependence of the eigenstates arising from the complex interplay of the *orbitals*, including atomic orbitals, spin, sites within the unit cells, and other potential quantum numbers relevant in the system under investigation.

A natural way to form scalar observables is to take traces of products of projectors, e.g.,

$$\text{tr}[\hat{P}_1(\mathbf{k}_1) \hat{P}_2(\mathbf{k}_2) \hat{P}_1(\mathbf{k}_3) \hat{P}_3(\mathbf{k}_4)], \quad (12)$$

involving multiple projectors of the same or different subsets and momenta. In the two cases we consider as applications in Secs. III A and III B, e.g., the polarization distribution and optical responses, the final expression involves projector combinations at only a single momentum $\mathbf{k}$ in combination with derivatives of the projectors, e.g.,

$$\text{tr}[\hat{P}_1(\mathbf{k}) (\partial_a \hat{P}_2(\mathbf{k})) (\partial_b \hat{P}_1(\mathbf{k})) (\partial_{c_1} \partial_{c_2} \partial_{c_3} \hat{P}_3(\mathbf{k}))]. \quad (13)$$

Expressions like Eq. (12) involving projectors at arbitrarily separated points on the Brillouin zone are called *global geometric invariants*. Expressions like Eq. (13) involving derivatives of projectors, that is, only infinitesimally separated in $\mathbf{k}$, are called *local geometric invariants*. Both should yield a complete characterization of the Bloch states with some caveats in the case of local invariants [12]. The goal of *quantum state geometry* is to identify all independent structures and their relationships. One of the main objectives is to identify the minimal number of structures that can appear in a specified physical context, such as optical responses and polarization distribution.

D. Intrinsic and extrinsic geometry

When determining the minimal set of independent geometric structures, it is essential to identify relations between different geometric objects. We would like to point out that these relations depend on whether the whole manifold of possible quantum states for a given number of bands is considered or just its submanifold made up by the state corresponding to the Bloch states, that is, those states in the whole manifold that are in the image of the projector $\hat{P}(\mathbf{k})$. This distinction becomes relevant when the (real) dimension of the complex projective space formed by all possible states is larger than the dimension of the Brillouin zone, i.e., $2(N-1) > d$ with N bands in d dimensions for a nondegenerate band.

This aspect is well established in Euclidean geometry, e.g., for surfaces in $\mathbb{R}^3$. At every point, the surface is described by two principal curvatures. Since they do not change under

isometries, they are individual geometric invariants of the surface embedding into the three-dimensional space. However, only the product of the curvatures is intrinsic to the surface, i.e., it can be reconstructed from the induced metric of $\mathbb{R}^3$ onto the surface. Thus embedding is crucial when characterizing the geometry, which can give rise to further geometric invariants.

We refer to the geometric invariants on the ambient space—the manifold of all possible quantum states—as *intrinsic* and all other geometric information, which characterizes the embedding, as *extrinsic*. In Ref. [12], it was shown for a single nondegenerate projector that the only intrinsic object is the quantum geometric tensor and objects of the form with second- and higher-order derivatives completely characterize the remaining extrinsic geometry; see Eqs. (16) and (15). The intrinsic objects for degenerate states are described in Sec. II F 5. The geometry of multistate objects is not yet sufficiently understood for separation into intrinsic and extrinsic invariants. Progress can be made by considering a Taylor expansion of global geometric invariants to identify those that fully describe the embedding.

E. Minimal quantum geometric structures

If only a single nondegenerate band $\hat{P}_m$ with band index m is involved, it was shown by one of us [12] that all global geometric invariants can be reduced to three-point functions of the form

$$\text{tr}[\hat{P}_m(\mathbf{k}_1)\hat{P}_m(\mathbf{k}_2)\hat{P}_m(\mathbf{k}_3)] \quad (14)$$

involving band projectors at three distinct momenta. Furthermore, all local geometric invariants reduce to a series of objects of the form

$$\mathcal{Q}_{\alpha;\beta_1\dots\beta_n}(\mathbf{k}) \equiv \text{tr}[\hat{P}(\mathbf{k})(\partial_\alpha\hat{P}(\mathbf{k}))(\partial_{\beta_1}\dots\partial_{\beta_n}\hat{P}(\mathbf{k}))] \quad (15)$$

involving the band projector and its first-order and n th derivative. Note that by construction $\mathcal{Q}_{\alpha;\beta_1\dots\beta_n}$ is symmetric in the β_i indices. In contrast, similar statements for degenerate bands and multistate quantum geometric structures involving projectors of multiple bands are more elaborate. A recent analysis by one of us showed that three-point functions are still sufficient for a single M -times degenerate band but show a much richer internal structure [13]. The part of the relevant structure discussed in the joint submission [7] and throughout this paper comes from Slater determinants and is equivalent to the nondegenerate case via Plücker embedding; see Sec. III A. A complete understanding of the quantum geometric structure of multistate (multiband) observables is still missing but is highly relevant for applications. For example, resonant optical responses involve two bands $\hat{P}_n$ and $\hat{P}_m$ when their band dispersions are on resonance, i.e., when $E_n(k) - E_m(k) = \omega$. New geometric objects have been identified and studied [23,27,34] in line with the discussion presented in the joint submission [7]. Despite recent progress, a comprehensive description is still lacking.

F. Important geometric invariants

We summarize several geometric invariants that have recently attracted attention and write them in projector form.

We provide a summary in Table I. We start with the quantum geometric tensor, involving the quantum metric and Berry curvature, and its multistate variant. We continue with the quantum geometric connection, relevant for the third cumulant, or skewness, of the polarization distribution and the shift current, as introduced in the joint submission [7], and the quantum metric and Berry curvature dipoles. We conclude by stressing the relation to the torsion tensor, a geometric quantity in systems with at least three bands [23,27]. Since we only focus on local geometric invariants, we introduce the short notation $\hat{P} \equiv \hat{P}(\mathbf{k})$, omitting the momentum dependence of the projector.

1. Quantum geometric tensor

The (*single-state*) quantum geometric tensor in projector form reads

$$\mathcal{Q}_{\alpha\beta} \equiv \text{tr}[\hat{P}(\partial_\alpha\hat{P})(\partial_\beta\hat{P})] \quad (16)$$

involving a projector onto a (non)degenerate band, occupied states, or other sets of quantum states. Besides the quantum geometric tensor expressed in the Bloch states for a nondegenerate band, see Appendix C, the projector form (16) has been extensively used in recent years, for instance, in the context of fractional quantum Hall physics; see, e.g., Refs. [10,35,36]. Decomposing the quantum geometric tensor into its symmetric and antisymmetric part with respect to the tensor indices α and β or, equivalently, into its real and imaginary part, we identify the quantum metric $g_{\alpha\beta}$ and Berry curvature $\Omega_{\alpha\beta}$ associated with the projector $\hat{P}$ as

$$\mathcal{Q}_{\alpha\beta} = g_{\alpha\beta} - \frac{i}{2}\Omega_{\alpha\beta}, \quad (17)$$

with

$$g_{\alpha\beta}(\mathbf{k}) \equiv \frac{1}{2}\text{tr}[(\partial_\alpha\hat{P})(\partial_\beta\hat{P})], \quad (18)$$

$$\Omega_{\alpha\beta}(\mathbf{k}) \equiv i\text{tr}[\hat{P}(\partial_\alpha\hat{P})(\partial_\beta\hat{P}) - \hat{P}(\partial_\beta\hat{P})(\partial_\alpha\hat{P})]. \quad (19)$$

We emphasize that the choice of quantum states of interest via the projector defines the quantum geometric tensor and, thus, the quantum metric and Berry curvature. The quantities for different projectors are generally not simply related; see, e.g., for the quantum metric of individual bands and the occupied states [11,37].

As the first multistate geometric invariant, we introduce the *two-state quantum geometric tensor*, which naturally generalizes the expression (16),

$$\mathcal{Q}_{\alpha\beta}^{mn} \equiv \text{tr}[\hat{P}_n(\partial_\alpha\hat{P}_m)(\partial_\beta\hat{P}_n)], \quad (20)$$

involving two (potentially) distinct projectors $\hat{P}_n$ and $\hat{P}_m$, usually referring to projectors on two different bands. For this, note the difference in the index of the middle projector. The decomposition of the two-state quantum geometric tensor in analogy to Eq. (17) into its symmetric and antisymmetric contribution naturally generalizes the quantum metric and Berry curvature to their two-state quantities, i.e.,

$$\mathcal{Q}_{\alpha\beta}^{mn} = g_{\alpha\beta}^{mn} - \frac{i}{2}\Omega_{\alpha\beta}^{mn}, \quad (21)$$

with

$$g_{\alpha\beta}^{mn} \equiv \frac{1}{2} \text{tr}[(\partial_\alpha \hat{P}_m(\mathbf{k}))(\partial_\beta \hat{P}_n(\mathbf{k}))], \quad (22)$$

$$\Omega_{\alpha\beta}^{mn} \equiv i \text{tr}[\hat{P}_n(\partial_\alpha \hat{P}_m)(\partial_\beta \hat{P}_n) - \hat{P}_n(\partial_\beta \hat{P}_m)(\partial_\alpha \hat{P}_n)]. \quad (23)$$

We note that the two-state quantum geometric tensor decomposes into the diagonal part given by the single-state quantum geometric tensor given in Eq. (16) and a purely two-state contribution,

$$Q_{\alpha\beta}^{mn} = \delta_{nm} Q_{\alpha\beta}^n - \text{tr}[\hat{e}_\alpha^{nm} \hat{e}_\beta^{mn}], \quad (24)$$

which we expressed in terms of

$$\hat{e}_\alpha^{mn} \equiv i \hat{P}_m(\partial_\alpha \hat{P}_n) \hat{P}_n. \quad (25)$$

Note that $\hat{e}_\alpha^{nn} = 0$ individually, which follows from projector identity (4). The purely two-state contribution $\text{tr}[\hat{e}_\alpha^{nm} \hat{e}_\beta^{mn}]$ yields the product of non-Abelian Berry connections, see Appendix C, and is, thus, directly connected to interband transitions in optical responses [23]. Using the completeness of the band projectors (6), the single- and two-state quantum geometric tensor are related via

$$\sum_{m \neq n} Q_{\alpha\beta}^{mn} = -Q_{\alpha\beta}^n. \quad (26)$$

Note that the negative-sign convention of the two-state quantum geometric tensor for $n \neq m$ arises from the form given in Eq. (20) fixing the relation $Q_{\alpha\beta}^{nn} = Q_{\alpha\beta}^n$ via the commonly used definition in Eq. (16). We conclude by noticing that $g_{\alpha\beta}^{mn} = g_{(\alpha\beta)}^{(mn)}$ and $\Omega_{\alpha\beta}^{mn} = \Omega_{[\alpha\beta]}^{[mn]}$ for $n \neq m$, where we denote the symmetrization and antisymmetrization of the indices as $(\alpha\beta)$ and $[\alpha\beta]$, respectively. Thus the symmetry with respect to the momentum derivative imposes the symmetry with respect to the band indices, which offers straightforward simplifications in analytic calculations [7, 11].

2. Quantum geometric connection

We continue by considering the second local geometric invariant in Eq. (15). For a given projector $\hat{P}$ we have the (single-state) quantum geometric connection

$$Q_{\alpha;\beta\gamma} \equiv \text{tr}[\hat{P}(\partial_\alpha \hat{P})(\partial_\beta \partial_\gamma \hat{P})], \quad (27)$$

which involves a first- and second-order derivative of the projector. Note that $Q_{\alpha;\beta\gamma} = Q_{\alpha;\gamma\beta}$. The quantum geometric connection is a complex-valued three-tensor and, therefore, is expected to yield a more complex structure than the quantum geometric tensor and further independent geometric information about the quantum states. As shown in Ref. [12] by one of us, and extended to degenerate bands in the joint submission [7], the imaginary part of $Q_{\alpha;\beta\gamma}$ is related to the third cumulant of the polarization distribution $\langle \hat{X}_\alpha \hat{X}_\beta \hat{X}_\gamma \rangle_c$ under integration over the Brillouin zone (BZ); see details in Sec. III A. We note that

$$\text{Im} Q_{\alpha;\beta\gamma} = \text{Im} Q_{(\alpha;\beta\gamma)} - \frac{1}{6}(\partial_\beta \Omega_{\alpha\gamma} + \partial_\gamma \Omega_{\alpha\beta}), \quad (28)$$

which follows from vanishing combinations of projector derivatives; see identities in Sec. II G 2. Thus we find $\int_{\text{BZ}} \text{Im} Q_{\alpha;\beta\gamma} = \int_{\text{BZ}} \text{Im} Q_{(\alpha;\beta\gamma)}$ since the boundary contribution involving the Berry curvature $\Omega_{\alpha\beta}$ vanishes. As Eq. (28) suggests, the quantum geometric connection contains the

quantum metric dipole and Berry curvature dipole. Indeed, we have

$$\partial_\alpha g_{\beta\gamma} = \text{Re}[Q_{\beta;\alpha\gamma} + Q_{\gamma;\alpha\beta}], \quad (29)$$

$$\partial_\alpha \Omega_{\beta\gamma} = -2 \text{Im}[Q_{\beta;\alpha\gamma} - Q_{\gamma;\alpha\beta}] \quad (30)$$

under symmetrization with respect to the first and last index of the quantum geometric connection. The quantum metric and Berry curvature dipole have been related, e.g., to nonlinear transport in a topological antiferromagnet [38] and the quantum nonlinear Hall effect [39], respectively.

As for the quantum geometric tensor, we present the multistate generalization of Eq. (27) and define the two-state quantum geometric connection

$$C_{\alpha;\beta\gamma}^{mn} \equiv \text{tr}[\hat{P}_n(\partial_\beta \hat{P}_m)[(\partial_\alpha \partial_\gamma \hat{P}_n) + (\partial_\alpha \hat{P}_m)(\partial_\gamma \hat{P}_n)]], \quad (31)$$

which involve a second-order derivative in combination with the product of three first-order derivatives of the projectors in a particular combination of indices n and m , usually related to band indices. This second term vanishes in the single-state (band-diagonal) component, see Sec. II G 2, so that $C_{\alpha;\beta\gamma}^{nn} = Q_{\alpha;\beta\gamma}^n$ given in Eq. (27) with respect to the band projector $\hat{P}_n$. This identification fixes our sign convention. We express the purely two-state (interband) component in terms of $\hat{e}_\alpha^{nm}$ and its covariant derivative $\nabla_\alpha \hat{e}_\gamma^{mn} \equiv \hat{P}_m(\partial_\alpha \hat{e}_\gamma^{mn}) \hat{P}_n$ as introduced in Ref. [23] and find

$$C_{\alpha;\beta\gamma}^{mn} = \delta_{nm} Q_{\beta;\alpha\gamma}^n - \text{tr}[\hat{e}_\beta^{nm} \nabla_\alpha \hat{e}_\gamma^{mn}]. \quad (32)$$

This form highlights the connection to higher-order optical responses as presented by Ahn *et al.* [23], where they interpreted transition dipole moment matrix elements as tangent vectors $\hat{e}_\alpha^{mn}$ with projector form given in Eq. (25).

We have a closer look at the tensor properties of the two-state quantum geometric connection. When decomposing $C_{\alpha;\beta\gamma}^{mn}$ for $n \neq m$ uniquely into its symmetric and antisymmetric components with respect to the band indices and two last derivative directions, we find that $C_{\alpha;(\beta\gamma)}^{(mn)}$ and $C_{\alpha;[\beta\gamma]}^{[mn]}$ are proportional to the dipole of the two-state quantum metric (22) and Berry curvature (23), respectively. The remaining $C_{\alpha;[\beta\gamma]}^{(mn)}$ and $C_{\alpha;(\beta\gamma)}^{[mn]}$ determine the shift current under linear and circular polarized illumination, respectively; see Ref. [7] and Sec. III B for a detailed discussion. The real and imaginary parts of $C_{\alpha;\beta\gamma}^{mn}$ are symmetric and antisymmetric in the band indices for $n \neq m$, respectively. We conclude by noticing that the summation over the off-diagonal band indices is not simply related to the single-state quantum geometric connection but yields a second term, i.e.,

$$\sum_{m \neq n} C_{\alpha;\beta\gamma}^{mn} = -Q_{\beta;\alpha\gamma}^n + \text{tr} \left[\hat{P}_n \left(\sum_{m \neq n} (\partial_\beta \hat{P}_m)(\partial_\alpha \hat{P}_m) \right) (\partial_\gamma \hat{P}_n) \right], \quad (33)$$

in contrast to the two-state quantum geometric tensor in Eq. (26). Note that the second term arises only in systems with more than two bands and vanishes in a two-band system; see Sec. II G 2.

Single-state four-derivative objects have been considered in [40, 41].

3. Torsion tensor

The torsion, as part of the two-state quantum geometric connection, captures geometric information about the Bloch state manifold arising in systems with more than two bands. Following our insights presented in the joint submission [7], we introduce the *torsion tensor* in projector form as

$$T_{\beta;\alpha\gamma}^{mn} \equiv \text{tr}[\hat{P}_n(\partial_\beta \hat{P}_m)(\partial_\alpha \hat{P}_m)(\partial_\gamma \hat{P}_n)] - (\alpha \leftrightarrow \gamma), \quad (34)$$

where we denote antisymmetrization in α and γ as the second term. This form agrees with the original definition [23] in terms of the tangent vector $\hat{e}_\alpha^{mn}$ using Eq. (25),

$$T_{\beta;\alpha\gamma}^{mn} = \text{tr}[\hat{e}_\beta^{nm}(\nabla_\alpha \hat{e}_\gamma^{mn} - \nabla_\gamma \hat{e}_\alpha^{mn} - [\hat{e}_\gamma^{mn}, \hat{e}_\alpha^{mn}])] \quad (35)$$

and is related to the antisymmetrization in the first and last index of the two-state quantum geometric connection, i.e.,

$$T_{\beta;\alpha\gamma}^{mn} = C_{\gamma;\beta\alpha}^{mn} - C_{\alpha;\beta\gamma}^{mn}. \quad (36)$$

Note that the torsion tensor vanishes for $n = m$ as well as for two-band systems as follows from the projector identity (4) and (6); see Sec. II G 2.

A cyclic summation of $C_{\alpha;\beta\gamma}^{(mn)}$ is proportional to the real part of the cyclic summation of the torsion tensor $T_{\alpha;\beta\gamma}^{mn}$, which relates the torsion tensor to the circular shift current and offers a different path for quantized nonlinear optical responses [27,42].

4. Interband Wilson loop and shift vector

We present the connection between the projector formalism and the gauge-invariant Pancharatnam-Berry phase over an interband loop, which has recently been introduced in the shift vector description of the shift current response [43–45]. The *interband Wilson loop* reads

$$W_{\alpha\beta}^{mn}(\mathbf{k}, \mathbf{q}) = \text{tr}[\hat{e}_\beta^{nm}(\mathbf{k}) \hat{e}_\alpha^{mn}(\mathbf{k} + \mathbf{q})] \quad (37)$$

involving the transition dipole moments in Eq. (25) at separated momenta. Note that the interband Wilson loop vanishes for $n = m$. It reduces to the established definition [44] for nondegenerate bands; see Appendix C 3. Expanding in small $\mathbf{q}$ leads to the two-state quantum geometric tensor and quantum geometric connection,

$$W_{\alpha\beta}^{mn}(\mathbf{k}, \mathbf{q}) = -Q_{\beta\alpha}^{mn}(\mathbf{k}) - \sum_\gamma q_\gamma C_{\gamma;\beta\alpha}^{mn}(\mathbf{k}) + \dots \quad (38)$$

Using Eq. (37), we derive the shift vector obtaining

$$R_{\alpha\beta}^{mn}(\mathbf{k}) \equiv i \lim_{q_a \rightarrow 0} \partial_{q_a} \ln W_{\beta\beta}^{mn}(\mathbf{k}, \mathbf{q}) = i \frac{C_{\alpha;\beta\beta}^{mn}(\mathbf{k})}{Q_{\beta\beta}^{mn}(\mathbf{k})}, \quad (39)$$

which reduces to the well-known expression [23,43–46] for nondegenerate bands; see Appendix C 3. In particular, we have

$$\text{Re } R_{\alpha\beta}^{mn} = -\frac{\text{Im } C_{\alpha;\beta\beta}^{mn}}{g_{\beta\beta}^{mn}}, \quad (40)$$

$$\text{Im } R_{\alpha\beta}^{mn} = \frac{\text{Re } C_{\alpha;\beta\beta}^{mn}}{g_{\beta\beta}^{mn}}, \quad (41)$$

which offers the interpretation of the shift vector as the metric-normalized quantum geometric connection.

5. Non-Abelian quantum geometric tensor

A single m -degenerate state is represented by a projector $\hat{P}$ of rank m . While one can still define the quantum geometric tensor according to Eq. (16), it does not exhaust all geometric information contained in the projector. A convenient way of representing the additional information is by considering its non-Abelian version,

$$\mathcal{Q}_{\alpha\beta}^{ab} = \langle u_a | (\partial_\alpha \hat{P})(\partial_\beta \hat{P}) | u_b \rangle, \quad (42)$$

with Bloch states $|u_a\rangle$ of the m -dimensional subspace. We denote this $m \times m$ matrix for fixed α, β as $\mathcal{Q}_{\alpha\beta}$ suppressing the internal indices. The Abelian quantum geometric tensor in Eq. (16) is recovered by tracing its non-Abelian version, i.e., $Q_{\alpha\beta} = \text{tr } \mathcal{Q}_{\alpha\beta}$.

The antisymmetric part of $\mathcal{Q}_{\alpha\beta}$ relates to the non-Abelian Berry curvature

$$F_{\alpha\beta} = i(\mathcal{Q}_{\alpha\beta} - \mathcal{Q}_{\beta\alpha}) \quad (43)$$

$$= \partial_\alpha A_\beta - \partial_\beta A_\alpha - [A_\alpha, A_\beta], \quad (44)$$

where A_α is the non-Abelian Berry connection, also known as the Wilczek-Zee connection. It is important to point out that, for $m > 1$, A_α cannot be recovered from $F_{\alpha\beta}$. We note that the trace of $F_{\alpha\beta}$ reduces to the Abelian Berry curvature given in Eq. (19). The symmetric part gives a matrix-valued generalization of the quantum metric,

$$G_{\alpha\beta} = \frac{1}{2}(\mathcal{Q}_{\alpha\beta} + \mathcal{Q}_{\beta\alpha}), \quad (45)$$

which is an intrinsic geometric invariant that, among other things, leads to a series of Finsler metrics

$$g_{\alpha_1\beta_1 \dots \alpha_n\beta_n}^{(n)} = \text{tr}[G_{(\alpha_1\beta_1} \dots G_{\alpha_n\beta_n)}], \quad (46)$$

for $n = 1, \dots, m$ with $g_{\alpha\beta}^{(1)}$ being the quantum metric given in Eq. (18). For $n > 1$, Eq. (46) yields independent ways of measuring the distance between degenerate states, corresponding to Jordan's principle angles. It was shown in Ref. [13] by one of us that A_α and $G_{\alpha\beta}$ give a full characterization of the intrinsic geometry of rank- m projectors. Physical observables will be expressed via traces or other scalar functions of these matrix-valued objects.

G. Useful projector identities

An efficient evaluation of geometric invariants involving multiple projectors and their derivatives require a set of identities, which are implied by the four basic projector properties given in Eqs. (3) to (6). We focus on those identities relevant for the evaluations throughout this paper and the joint submission [7]. Further generalizations are straightforwardly obtained. We omit the momentum dependence throughout this section, i.e., $\hat{P} \equiv \hat{P}(\mathbf{k})$.

1. Trace manipulations and complex conjugation

The cyclic property of the trace allows the cyclic permutation of the involved projectors,

$$\text{tr}[\hat{P}_1 \hat{P}_2 \dots \hat{P}_N] = \text{tr}[\hat{P}_2 \dots \hat{P}_N \hat{P}_1], \quad (47)$$

and further operators such as the Bloch Hamiltonian. The invariance of the trace under transposition and the Hermiticity

of the projectors (3) lead to

$$\overline{\text{tr}[\hat{P}_1 \hat{P}_2 \dots \hat{P}_N]} = \text{tr}[\hat{P}_N \dots \hat{P}_2 \hat{P}_1], \quad (48)$$

where the overline denotes complex conjugation. We note that complex conjugation effectively reverses the order of the projectors under the trace. The same identity holds when projector derivatives and other Hermitian operators are involved. The two trace manipulations (47) and (48) are essential in the evaluation of diagrammatic expansions; see, e.g., Ref. [47] and Sec. III B.

2. Vanishing projector combinations

The idempotence and orthogonality of the projectors formalized in the identity (4) directly implies

$$\partial_\alpha \hat{P} = \hat{P} (\partial_\alpha \hat{P}) + (\partial_\alpha \hat{P}) \hat{P}. \quad (49)$$

Note that the projector and its derivative do not commute in general. This identity implies the vanishing of the following three combinations of projector and their derivatives:

$$\hat{P} (\partial_\alpha \hat{P}) \hat{P} = 0, \quad (50)$$

$$\hat{P} (\partial_\alpha \hat{P}) (\partial_\beta \hat{P}) (\partial_\gamma \hat{P}) \hat{P} = 0, \quad (51)$$

$$\text{tr}[(\partial_\alpha \hat{P}) (\partial_\beta \hat{P}) (\partial_\gamma \hat{P})] = 0. \quad (52)$$

Note that the last identity is only valid under the trace. The upper identities are proven by inserting (49) repetitively for all derivatives, which allows for a systematic derivation of further vanishing projector identities beyond the presented ones. Projector identities with higher-order derivatives can be derived using $\partial_{\alpha_1} \dots \partial_{\alpha_n} \hat{P} = \partial_{\alpha_n} \dots \partial_{\alpha_1} \hat{P}^2$. Extending the derivation to projectors of different bands, it immediately follows from (4) that

$$\hat{P}_m (\partial_\alpha \hat{P}_l) \hat{P}_n = 0 \quad (53)$$

for $l \neq n, m$.

3. Derivatives of the Bloch Hamiltonian

In the derivation of response functions, derivatives of the Bloch Hamiltonian are usually present. We summarize the most important identities arising from projector property (5) or, equivalently,

$$\hat{H} = \sum_n E_n \hat{P}_n, \quad (54)$$

where we omit the momentum dependence of the band dispersions $E_n \equiv E_n(\mathbf{k})$ and the corresponding band projectors $\hat{P}_n \equiv \hat{P}_n(\mathbf{k})$ for shorter notation. We obtain

$$\hat{P}_m (\partial_\alpha \hat{H}) \hat{P}_n = \delta_{mn} (\partial_\alpha E_m) \hat{P}_m - \epsilon_{mn} \hat{P}_m (\partial_\alpha \hat{P}_n) \hat{P}_n, \quad (55)$$

with direct band gaps $\epsilon_{mn} \equiv E_m - E_n$, where we used Eq. (53) and $\hat{P}_m (\partial_\alpha \hat{P}_m) \hat{P}_n = -\hat{P}_m (\partial_\alpha \hat{P}_n) \hat{P}_n$. Similarly, we obtain the decomposition of the second-order Hamiltonian derivative

$$\begin{aligned} \hat{P}_m (\partial_\alpha \partial_\beta \hat{H}) \hat{P}_n &= \frac{1}{2} \epsilon_{nm} \hat{P}_m (\partial_\alpha \partial_\beta \hat{P}_n) \hat{P}_n + (\partial_\alpha \epsilon_{nm}) \hat{P}_m (\partial_\beta \hat{P}_n) \hat{P}_n \\ &\quad - E_m \hat{P}_m (\partial_\alpha \hat{P}_m) (\partial_\beta \hat{P}_n) \hat{P}_n \\ &\quad - \sum_{l \neq n, m} E_l \hat{P}_m (\partial_\alpha \hat{P}_l) \hat{P}_l (\partial_\beta \hat{P}_n) \hat{P}_n + (\alpha \leftrightarrow \beta) \end{aligned} \quad (56)$$

for $n \neq m$, where the symmetry in α and β are denoted in the last line.

4. Two-band systems

We have a closer look at the case of a two-band system with nondegenerate bands, which are highly constrained via the completeness relation (6), i.e.,

$$\hat{P}_+ + \hat{P}_- = \mathbb{1}_2, \quad (57)$$

where we denote the two band projectors as $\hat{P}_\pm$. This relation implies $\partial_\alpha \hat{P}_+ = -\partial_\alpha \hat{P}_-$ and, thus, greatly simplifies the geometric invariants. In particular, we have

$$g_{\alpha\beta}^{+-} = -g_{\alpha\beta}^- = -g_{\alpha\beta}^+ = g_{\alpha\beta}^{--}, \quad (58)$$

$$\Omega_{\alpha\beta}^{+-} = -\Omega_{\alpha\beta}^- = \Omega_{\alpha\beta}^+ = -\Omega_{\alpha\beta}^{--}, \quad (59)$$

relating the quantum metric, Berry curvature, and their two-state variants of the two bands. We see that only a single quantum metric and Berry curvature determine all quantities.

Similarly, we obtain the relation between the different components of the quantum geometric connections

$$C_{\alpha;\beta\gamma}^{+-} = -Q_{\beta;\alpha\gamma}^- = -\overline{Q_{\beta;\alpha\gamma}^+} = \overline{C_{\alpha;\beta\gamma}^{--}}, \quad (60)$$

where the overline denotes complex conjugation. These relations imply that the torsion of a two-band system vanishes, i.e.,

$$T_{\beta;\alpha\gamma}^{+-} = C_{\gamma;\beta\alpha}^{+-} - C_{\alpha;\beta\gamma}^{+-} = -Q_{\beta;\gamma\alpha}^- + Q_{\beta;\alpha\gamma}^- = 0. \quad (61)$$

We can generalize these insights to any separation of the entire system into two subsystems, for instance, the set of occupied and unoccupied states characterized by $\hat{P}_{\text{occ}}$ and $\hat{P}_{\text{unocc}} = \mathbb{1}_N - \hat{P}_{\text{occ}}$.

Note that the relations above can also be seen as a consequence of Eqs. (26) and (33) for a two-band system. However, this does not generalize to arbitrary subsets. As we discuss in the joint submission [7], the summed-over two-state quantum geometric connection $\sum_{n \in \text{occ}} \sum_{m \in \text{unocc}} C_{\alpha\beta}^{mn}$ does not, in general, reduce to a ground state property, i.e., cannot that can be expressed using $\hat{P}_{\text{occ}}$ only.

III. APPLICATIONS OF THE FORMALISM

We present two applications of the formalism described in Sec. II, which both provide further physical insights into the quantum geometric invariants and illustrate how derivations of observables and their relation to geometric invariants are performed within the projector calculus. We start with the quantum state geometry of polarization in Sec. III A, which focuses on the single-state quantities, and close by the derivation of the injection and shift current in Sec. III B, which elaborates on the two-state quantities.

A. Quantum state geometry of polarization

In the first example, we focus on the polarization of extended periodic systems. We start by introducing the necessary concepts and formalism. The approach is known as the modern theory of polarization in the literature and was motivated by the need to define spontaneous polarization in

ferroelectrics rigorously [48,49]. The main challenge is that the naive definition of the polarization vector $\mathbf{P}$ via

$$\mathbf{P} = \int_{\text{sample}} d^d \mathbf{x} \, n(\mathbf{x}) \mathbf{x} \quad (62)$$

does not yield a well-defined bulk property due to corrections of the order of the sample volume $O(V_{\text{sample}})$ coming from adding charges at the boundary. One way to properly define bulk polarization is via a sum over Wannier functions $|W_n\rangle$ constructed from the occupied bands

$$\mathbf{P} = \sum_{n \in \text{occ}} \langle W_n | \hat{\mathbf{x}} | W_n \rangle, \quad (63)$$

with summation over the Wannier functions spanning all occupied bands. In the following, we take an alternative approach to deriving the average polarization and higher-order moments of the polarization distribution. For this, let us define the total (many-body) position operator on a lattice as $\hat{\mathbf{X}} = \sum_{i \in \text{sites}} \hat{\mathbf{x}}_i$, which is related to the polarization operator by $\hat{\mathbf{P}} = -e \hat{\mathbf{X}}$. The generating function for its moments reads

$$\begin{aligned} C(\mathbf{q}) &= \langle \Psi | e^{i\mathbf{q} \cdot \hat{\mathbf{X}}} | \Psi \rangle \\ &= 1 + i \sum_{\alpha} q_{\alpha} \langle \Psi | \hat{X}_{\alpha} | \Psi \rangle \\ &\quad - \frac{1}{2} \sum_{\alpha, \beta} q_{\alpha} q_{\beta} \langle \Psi | \hat{X}_{\alpha} \hat{X}_{\beta} | \Psi \rangle_c \\ &\quad + \frac{1}{6} \sum_{\alpha, \beta, \gamma} q_{\alpha} q_{\beta} q_{\gamma} \langle \Psi | \hat{X}_{\alpha} \hat{X}_{\beta} \hat{X}_{\gamma} | \Psi \rangle_c + \dots, \end{aligned} \quad (64)$$

where $|\Psi\rangle$ is the wave function of the electronic state and the subscript c stands for the connected correlator, which reads for the second and third cumulant,

$$\begin{aligned} \langle \hat{X}_{\alpha} \hat{X}_{\beta} \rangle_c &= \langle \hat{X}_{\alpha} \hat{X}_{\beta} \rangle - \langle \hat{X}_{\alpha} \rangle \langle \hat{X}_{\beta} \rangle, \\ \langle \hat{X}_{\alpha} \hat{X}_{\beta} \hat{X}_{\gamma} \rangle_c &= \langle \hat{X}_{\alpha} \hat{X}_{\beta} \hat{X}_{\gamma} \rangle - \langle \hat{X}_{\alpha} \hat{X}_{\beta} \rangle \langle \hat{X}_{\gamma} \rangle \\ &\quad - \langle \hat{X}_{\beta} \hat{X}_{\gamma} \rangle \langle \hat{X}_{\alpha} \rangle - \langle \hat{X}_{\gamma} \hat{X}_{\alpha} \rangle \langle \hat{X}_{\beta} \rangle + 2 \langle \hat{X}_{\alpha} \rangle \langle \hat{X}_{\beta} \rangle \langle \hat{X}_{\gamma} \rangle. \end{aligned} \quad (65)$$

In the noninteraction case, $|\Psi\rangle = \prod_{n, \mathbf{k}} u_n(\mathbf{k}) \hat{c}_{n\mathbf{k}}^{\dagger} |0\rangle$ is given by the Slater determinant constructed from the occupied states. As discussed in the following subsection, Slater determinants have the remarkable property of only depending on the subspace spanned by the participating states. We will develop an approach to describing the center-of-mass information in the Slater determinant in terms of the projector on all occupied bands, $\hat{P}_{\text{occ}}(\mathbf{k}) = \sum_{n \in \text{occ}} \hat{P}_n(\mathbf{k})$.

1. Slater determinants and the Plücker map

The Slater determinant is a natural way of constructing a many-body fermionic state out of a collection of m single-body states $|\psi_i\rangle$ via

$$\begin{aligned} \Psi(x_1, x_2, x_3, \dots) \\ = \frac{1}{m!} \det \begin{pmatrix} \psi_1(x_1) & \psi_2(x_1) & \psi_3(x_1) & \dots \\ \psi_1(x_2) & \psi_2(x_2) & \psi_3(x_2) & \dots \\ \psi_1(x_3) & \psi_2(x_3) & \psi_3(x_3) & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \end{aligned} \quad (67)$$

Due to the properties of the determinant, the set of states $U|\psi_i\rangle$, where U is a unitary, gives the same state modulo a phase. Thus the resulting state is a function of $\text{span}\{|\psi_i\rangle\}$ only. This construction is known as the Plücker map in mathematics. Formally, it is a map from the Grassmannian $\text{Gr}(m, V)$, the space of m planes in V , to the projectivization of the exterior power of the original vector space $P(\Lambda^m V)$. In physical terms, the exterior power $\Lambda^m V$ is the many-body fermionic Hilbert space. Explicitly, the Plücker map is given by

$$\text{span}(w_1, \dots, w_m) \rightarrow [w_1 \wedge \dots \wedge w_m], \quad (68)$$

where $\wedge$ stands for the exterior product and $[\dots]$ stands for projectivization. We use this map to define the geometric objects associated with a single state of an entire subspace. The starting point is the inner product that is induced on the exterior power

$$\langle \Lambda v, \Lambda w \rangle = \det(\langle v_i | w_j \rangle) \quad (69)$$

with the matrix $(\langle v_i | w_j \rangle)$ involving all combinations of the single-particle states within the many-body states Λv and Λw . With that, given three m -dimensional subspaces spanned by $|v_i\rangle$, $|w_i\rangle$, and $|u_i\rangle$, we define the three-point function [12] via

$$\begin{aligned} \langle \Lambda v, \Lambda w \rangle \langle \Lambda w, \Lambda u \rangle \langle \Lambda u, \Lambda v \rangle \\ = \det(\langle v_i | w_j \rangle) \det(\langle w_i | u_j \rangle) \det(\langle u_i | v_j \rangle) \\ = \sum_{s, s'} \det(\langle v_i | w_s \rangle \langle w_s | u_{s'} \rangle \langle u_{s'} | v_j \rangle), \end{aligned} \quad (70)$$

where we used $\det(AB) = \det A \det B$. We can alternatively write it as

$$\det_v [\hat{P}_v \hat{P}_w \hat{P}_u \hat{P}_v], \quad (71)$$

where $\hat{P}_v = \sum_s |v_s\rangle \langle v_s|$ (and analogously for w and u) and $\det_v$ is taken over the $\hat{P}_v$ subspace. Considering that $\{v_s\}$ forms a basis of the image $\text{Im } \hat{P}_v$, we need to compute $\langle v_s | \hat{P}(w) \hat{P}(u) | v_s \rangle$. We keep the last projector to make the projection onto the subspace explicit. The described procedure allows us to generalize the geometric characterization of the $\mathbb{C}P^n$ theory as presented in Ref. [12] by one of us to invariants that can be written as

$$\det_{v_1} [\hat{P}_{v_1} \hat{P}_{v_2} \dots \hat{P}_{v_m} \hat{P}_{v_1}]. \quad (72)$$

In particular, all invariants of that form can be reduced to three-point functions such as given in Eq. (70).

2. Polarization

Consider an insulator with N_{occ} filled bands. The corresponding ground state wave function is $|\Psi\rangle = \prod_{n, \mathbf{k}} u_n(\mathbf{k}) \hat{c}_{n\mathbf{k}}^{\dagger} |0\rangle$ with vacuum $|0\rangle$ and fermionic creation operators $\hat{c}_{n\mathbf{k}}^{\dagger}$. We notice that $e^{i\mathbf{q} \cdot \hat{\mathbf{X}}} |\Psi\rangle = \prod_{n, \mathbf{k}} u_n(\mathbf{k}) \hat{c}_{n, \mathbf{k}-\mathbf{q}}^{\dagger} |0\rangle$. Thus the generating function reads [50]

$$C(\mathbf{q}) \equiv \int_{\text{BZ}} \log \det(\langle u_i(\mathbf{k}) | u_j(\mathbf{k} + \mathbf{q}) \rangle)_{ij}, \quad (73)$$

where the determinant is taken over the matrix with entries $\langle u_i(\mathbf{k}) | u_j(\mathbf{k} + \mathbf{q}) \rangle$. In Appendix D, we redo the derivation from Ref. [12] for multiple filled bands. The resulting

expression is

$$\frac{\log C(\mathbf{q})}{V} = \sum_{\alpha} q^{\alpha} \mathcal{A}_{\alpha} + \sum_{\alpha} q^{\alpha} \int_{\text{BZ}} \int_0^1 dt \mathcal{A}_{\alpha}^{\mathbf{k}}(\mathbf{k} + \mathbf{q}t) \quad (74)$$

with the vector-valued two-point function

$$\mathcal{A}_{\alpha}^{\mathbf{k}}(\mathbf{k}') = \text{tr}[\hat{P}_{\mathbf{k}} (\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}'}^{-1} \hat{P}_{\mathbf{k}} (\partial_{\alpha} \hat{P}_{\mathbf{k}'} \hat{P}_{\mathbf{k}})]. \quad (75)$$

This result generalizes Eq. (17) in Ref. [12] to higher-rank projectors and was reported in the companion article [7]. The inversion operation $(\cdot)^{-1}$ is performed over the $\hat{P}_{\mathbf{k}}$ subspace. In the nondegenerate case, the product $\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}'} \hat{P}_{\mathbf{k}}$ is a rank-1 object so that the inverse is taken over a number. This number can be pulled out of the trace. Combining the rest in the trace and rewriting the number as a trace over the full space, we recover the rank-1 formula introduced in Ref. [12] up to complex conjugation, which we redefined for the convenience of a simpler notation. In the degenerate case, we can evaluate Eq. (75) by interpreting the objects as matrices within a particular basis. In particular, all operations are taken over the degenerate subspace only or the inverse can be expanded to the size of the original case after inversion restricted to the subspace by adding zero elements in the matrices.

The generating function in Eq. (74) allows us to derive the cumulants of polarization through the expansion of $\mathcal{A}_{\alpha}^{\mathbf{k}}(\mathbf{k} + \mathbf{q}t)$, that is,

$$\begin{aligned} \mathcal{A}_{\alpha}^{\mathbf{k}}(\mathbf{k} + \mathbf{q}) &= \sum_{\beta} Q_{\alpha\beta}(\mathbf{k}) q^{\beta} \\ &+ \sum_{\beta,\gamma} Q_{\alpha;\beta\gamma}(\mathbf{k}) q^{\beta} q^{\gamma} + \dots, \end{aligned} \quad (76)$$

where we identify the quantum geometric tensor and quantum geometric connection given in Eqs. (16) and (27) with respect to the projector onto the N_{occ} filled bands for the linear and quadratic term of the expansion, respectively. This leads to the explicit expressions for the second and third cumulants of the polarization distribution,

$$\langle X_{\alpha} X_{\beta} \rangle_c = V \int_{\text{BZ}} \text{Re} Q_{\alpha\beta}(\mathbf{k}), \quad (77)$$

$$\langle X_{\alpha} X_{\beta} X_{\gamma} \rangle_c = V \int_{\text{BZ}} \text{Im} Q_{\alpha;\beta\gamma}(\mathbf{k}), \quad (78)$$

as reported in the companion article [7]. We note that higher cumulants are, in general, not simply related to the single-state (nondegenerate) geometric invariants given in Eq. (15) by replacing the nondegenerate with the degenerate projectors. Instead, we expect deviations in the expansion of $\mathcal{A}_{\alpha}^{\mathbf{k}}(\mathbf{k} + \mathbf{q})$ between the nondegenerate and degenerate cases starting in the third order.

B. Injection and shift currents

We demonstrate the projector calculus for injection and shift currents, where the relevance of higher-order multistate quantum geometry, that is, the two-state quantum geometric tensor and the two-state quantum geometric connection, is known [23,25,26]. We explicitly show that the gauge invariance of the projector calculus allows for a straightforward

and transparent derivation despite the need to include various contributions that arise within the standard diagrammatic expansion. Within the projector formalism, unnecessary separations into gauge-dependent terms are avoided and the expressions are provided in a unified language that allows for simpler recombination of contributions from different diagrams.

We consider the second-order dc optical response

$$j^a(0; \omega, -\omega) = \sum_{b,c} \sigma^{a;bc}(0; \omega, -\omega) \mathcal{E}^b(\omega) \mathcal{E}^c(-\omega), \quad (79)$$

where $E^a(\omega)$ is the Fourier component of the external electric fields and j^a is the electric current. We will use the results of Ref. [25] which expressed $\sigma^{a;bc}$ in terms of the Bloch Hamiltonian $\hat{H}$. For a structured calculation, we split the conductivity into three parts distinct by the maximal order of the vertices from three to one, defining

$$\begin{aligned} \sigma^{a;bc}(\omega) &\equiv \sigma^{a;bc}(0, \omega, -\omega) \\ &= \frac{e^3}{\hbar^2 \omega^2} \int_{\text{BZ}} (\sigma_{(0)}^{a;bc} + \sigma_{(1)}^{a;bc}(\omega) + \sigma_{(2)}^{a;bc}(\omega)). \end{aligned} \quad (80)$$

For shorter notation, we do not explicitly write the momentum dependence within the integrand of the integral over the Brillouin zone (BZ). We focus on the contribution

$$\begin{aligned} \sigma_{(2)}^{a;bc}(\omega) &= \text{tr} \left[\hat{P}_{\text{occ}} \left(\left[\left[\partial_c \hat{H}, \frac{\partial_a \hat{H}}{\epsilon - i\gamma} \right], \frac{\partial_b \hat{H}}{\omega + \epsilon + i\Gamma} \right] \right. \right. \\ &\quad \left. \left. + \left[\left[\partial_b \hat{H}, \frac{\partial_a \hat{H}}{\epsilon - i\gamma} \right], \frac{\partial_c \hat{H}}{-\omega + \epsilon + i\Gamma} \right] \right) \right] \end{aligned} \quad (81)$$

involving only first-order vertices $\partial_a \hat{H}$ and present more details for the other two contributions in Appendix E. The individual terms are defined within the band basis, for instance, $\langle u_n | \partial_a \hat{H} / (-\epsilon + i\gamma) | u_m \rangle = \langle u_n | \partial_a \hat{H} | u_m \rangle / (-\epsilon_{nm} + i\gamma)$. We refer to Refs. [25,51] for a detailed physical motivation of the intraband relaxation rate γ and interband relaxation rate Γ . The numbers ω , γ , and Γ are understood to be multiplied with the identity matrix. $\epsilon_{nm} = E_n - E_m$ is the direct band gap between bands n and m . The $[\cdot, \cdot]$ is the commutator of the involved matrices. We simplified the notation given in Ref. [25] by introducing

$$\hat{P}_{\text{occ}} \equiv \sum_n f_n \hat{P}_n, \quad (82)$$

with Fermi function f_n and orthogonal band projector $\hat{P}_n$ with corresponding (non)degenerate band energy E_n . Note that $\hat{P}_{\text{occ}}$ is *not* a projector except for a band insulator at zero temperature but this close connection motivates us to introduce the notation. We do not need to assume that $\hat{P}_{\text{occ}}$ is a projector throughout the following derivation.

1. General strategy

Before performing the derivation in detail, we sketch the main steps, which we anticipate to apply to other observables as well, as long as the starting point is similar. We provided a detailed discussion on anticipated further applications of the formalism within the companion article [7]. Within the following derivation, we aim to separate quantum geometric

invariants that only involve projectors as introduced in Sec. II from a remaining part. This remaining spectral part usually captures the information about the band energies, temperature, or other external parameters. We perform this separation in an iterative process involving three main steps, which we illustrate for the injection and shift current in the following.

(Step 1) In order to evaluate the expression in Eq. (81), we first aim to separate the contributions involving spectral information such as the band energies, referred to as *spectral contribution*, from (preliminary) geometric contributions that might still contain spectral information. For this, we introduce projector expressions via Eqs. (6) and (54). It might be convenient to keep derivatives of the Hamiltonian explicit in order to avoid, at that point of the derivation, lengthy expressions arising from identities such as those given in Eqs. (55) and (56).

(Step 2) We use projector identities such as those presented in Sec. II G to simplify the individual (preliminary) geometric contributions, for instance, when performing the commutators. This generically leads to constraints for the band summations, further simplifying the spectral contribution.

(Step 3) We conclude by regrouping contributions with the same spectral contributions after the simplifications of the second step. Usually, further projector identities, as presented in Sec. II G, can be applied to obtain the final form, where we finally identify the relevant geometric invariant that only contains band projectors. In the following application to the injection and shift current, we know that the final result will involve only the quantities presented in Sec. II F. In general, other geometric invariants may be necessary to consider.

2. Step-by-step evaluation of Eq. (81)

We notice that it is sufficient to evaluate

$$B^{abc}(\omega) \equiv \text{tr} \left[\hat{P}_{\text{occ}} \left[\left[\partial_a \hat{H}, \frac{\partial_b \hat{H}}{\epsilon - i\gamma} \right], \frac{\partial_c \hat{H}}{\omega + \epsilon + i\Gamma} \right] \right], \quad (83)$$

since $\sigma_{(2)}^{a:bc}(\omega) = B^{cab}(\omega) + B^{bac}(-\omega)$. Following the first step of the general strategy, we focus on the two fractions involving the band energies. Using Eq. (54), we see that the contribution involving the interband relaxation rate Γ decomposes into

$$\begin{aligned} \frac{\partial_a \hat{H}}{\omega + \epsilon + i\Gamma} &= \sum_n \frac{\partial_a E_n}{\omega + i\Gamma} \hat{P}_n \\ &\quad - \sum_{\substack{n,m \\ n \neq m}} \frac{\epsilon_{nm}}{\omega + \epsilon_{nm} + i\Gamma} \hat{P}_n (\partial_a \hat{P}_m) \hat{P}_m, \end{aligned} \quad (84)$$

where we used Eq. (55) to evaluate the derivative of the Hamiltonian. Equivalently, we apply the same decomposition for the contribution involving the intraband relaxation rate γ and obtain

$$\frac{\partial_a \hat{H}}{\epsilon - i\gamma} = \frac{i}{\gamma} \sum_n (\partial_a E_n) \hat{P}_n - \sum_n \hat{Q}_n^{(\gamma)} (\partial_a \hat{P}_n) \hat{P}_n, \quad (85)$$

where we introduce

$$\hat{Q}_n^{(\gamma)} \equiv \sum_{m \neq n} \frac{\epsilon_{mn}}{\epsilon_{mn} - i\gamma} \hat{P}_m \approx \mathbb{1}_N - \hat{P}_n, \quad (86)$$

which projects onto the complement of band n in our limit of interest $\gamma \ll |\epsilon_{mn}|$. We see that we obtain four contributions when inserting Eqs. (84) and (85) into Eq. (83). We analyze the four contributions in the following. We notice that the four contributions involve two structures that simplify to

$$\text{tr}[\hat{P}_{\text{occ}}[\hat{O}, \hat{P}_n]] = 0, \quad (87)$$

$$\text{tr}[\hat{P}_{\text{occ}}[\hat{O}_1, \hat{P}_n \hat{O}_2 \hat{P}_m]] = -f_{nm} \text{tr}[\hat{O}_1 \hat{P}_n \hat{O}_2 \hat{P}_m], \quad (88)$$

using Eq. (82), which hold for arbitrary operators $\hat{O}$, $\hat{O}_1$, and $\hat{O}_2$.

Following the second step of our general strategy, we start with the term involving the first terms of Eq. (84) in combination with the first and second term of Eq. (85). Using the identity in Eq. (87), we see that both contributions vanish, i.e.,

$$\text{tr}[\hat{P}_{\text{occ}}[[\partial_a \hat{H}, \hat{P}_n], \hat{P}_{n'}]] = 0, \quad (89)$$

$$\text{tr}[\hat{P}_{\text{occ}}[[\partial_a \hat{H}, \hat{Q}_n^{(\gamma)} (\partial_b \hat{P}_n) \hat{P}_n], \hat{P}_{n'}]] = 0. \quad (90)$$

Combining the second term of Eq. (84) with the first term of Eq. (85) involves

$$- \text{tr}[\hat{P}_{\text{occ}}[[\partial_a \hat{H}, \hat{P}_n], \hat{P}_{n'} (\partial_c \hat{P}_{m'}) \hat{P}_{m'}]] \quad (91)$$

$$= f_{n'm'} \text{tr}[[\partial_a \hat{H}, \hat{P}_n] \hat{P}_{n'} (\partial_c \hat{P}_{m'}) \hat{P}_{m'}] \quad (92)$$

$$= (\delta_{nn'} - \delta_{nn'}) f_{n'm'} \text{tr}[(\partial_a \hat{H}) \hat{P}_{n'} (\partial_c \hat{P}_{m'}) \hat{P}_{m'}], \quad (93)$$

where we have used the basic projector property (4) to derive the constraint on the band summations. Collecting the spectral contributions and performing the band summations leads to

$$\frac{i}{\gamma} \sum_{\substack{n,m \\ n \neq m}} \frac{(\partial_b \epsilon_{nm}) \epsilon_{nm} f_{nm}}{\omega + \epsilon_{nm} + i\Gamma} \text{tr}[(\partial_a \hat{H}) \hat{P}_n (\partial_c \hat{P}_m) \hat{P}_m]. \quad (94)$$

The last term arising from Eq. (83) involves the second term of Eq. (84) in combination with the second term of Eq. (85). Using the approximation $\gamma \ll |\epsilon_{nm}|$ in Eq. (86), we obtain after similar steps

$$\begin{aligned} \sum_{\substack{n,m \\ n \neq m}} \frac{\epsilon_{nm} f_{nm}}{\omega + \epsilon_{nm} + i\Gamma} \text{tr}[(\partial_a \hat{H}) (\partial_b \hat{P}_n) \\ + (\partial_b \hat{P}_m) (\partial_a \hat{H})] \hat{P}_n (\partial_c \hat{P}_m) \hat{P}_m. \end{aligned} \quad (95)$$

Combining these results, we find that the contributions to the injection and shift current arising from the contributions involving three single-order vertices read

$$\begin{aligned} \sigma_{(2)}^{a:bc}(\omega) &= \sum_{\substack{n,m \\ n \neq m}} \tilde{s}_{nm}^{(1)}(\omega) \text{tr}[(\partial_c \hat{H}) \hat{P}_n (\partial_b \hat{P}_m) \hat{P}_m] \\ &\quad + \sum_{\substack{n,m \\ n \neq m}} \tilde{s}_{nm}^{(1)}(-\omega) \text{tr}[(\partial_b \hat{H}) \hat{P}_n (\partial_c \hat{P}_m) \hat{P}_m] \\ &\quad - \sum_{\substack{n,m \\ n \neq m}} \tilde{s}_{nm}^{(2)}(\omega) \text{tr}[(\partial_c \hat{H}) (\partial_a \hat{P}_n) + (\partial_a \hat{P}_m) (\partial_c \hat{H})] \hat{P}_n (\partial_b \hat{P}_m) \hat{P}_m \\ &\quad - \sum_{\substack{n,m \\ n \neq m}} \tilde{s}_{nm}^{(2)}(-\omega) \text{tr}[(\partial_b \hat{H}) (\partial_a \hat{P}_n) + (\partial_a \hat{P}_m) (\partial_b \hat{H})] \hat{P}_n (\partial_c \hat{P}_m) \hat{P}_m. \end{aligned} \quad (96)$$

We have introduced the short notation for the part of the spectral contributions that we have identified so far,

$$\tilde{s}_{nm}^{(1)}(\omega) \equiv \frac{i}{\gamma} \frac{(\partial_a \epsilon_{nm}) \epsilon_{nm} f_{nm}}{\omega + \epsilon_{nm} + i\Gamma}, \quad (97)$$

$$\tilde{s}_{nm}^{(2)}(\omega) \equiv \frac{\epsilon_{nm} f_{nm}}{\omega + \epsilon_{nm} + i\Gamma}. \quad (98)$$

As shown in Appendix D, the first contribution in Eq. (80) vanishes, $\sigma_{(0)}^{a;bc} = 0$, to leading order in $\gamma \ll |\epsilon_{nm}|$. The contribution to the injection and shift current involving both first- and second-order vertices reads

$$\begin{aligned} \sigma_{(1)}^{a;bc}(\omega) = & - \sum_{\substack{n,m \\ n \neq m}} \tilde{s}_{nm}^{(2)}(\omega) \text{tr}[(\partial_a \partial_c \hat{H}) \hat{P}_n (\partial_b \hat{P}_m) \hat{P}_m] \\ & + \sum_{\substack{n,m \\ n \neq m}} \tilde{s}_{nm}^{(2)}(-\omega) \text{tr}[(\partial_a \partial_b \hat{H}) \hat{P}_n (\partial_c \hat{P}_m) \hat{P}_m]. \end{aligned} \quad (99)$$

In light of the third step in our general strategy, we note that the contributions that are proportional to $\tilde{s}_{nm}^{(1)}$ cannot be further combined with other contributions. In contrast, several contributions involve $\tilde{s}_{nm}^{(2)}$ that we combine in the following.

3. Combining all contributions to identify the relevant geometric invariants

We start with the term that cannot be further reduced. Using the identity (55) to evaluate the derivative of the Bloch Hamiltonian and further simplify the resulting combinations of projectors via our results in Sec. II G 2, we identify the two-state quantum geometric tensor, i.e.,

$$\text{tr}[(\partial_c \hat{H}) \hat{P}_n (\partial_b \hat{P}_m) \hat{P}_m] = \epsilon_{nm} Q_{cb}^{nm}. \quad (100)$$

Note that the band diagonal contribution vanishes due to $\hat{P}_n (\partial_b \hat{P}_n) \hat{P}_n = 0$.

The contributions in Eq. (99) can be combined with those in Eq. (96) proportional to $\tilde{s}_{nm}^{(2)}$. Since the second derivative of the Bloch Hamiltonian is already given in Eq. (56), we focus only on the projector contributions in Eq. (96). Expanding the Bloch Hamiltonian in its projector representation leads to

$$\begin{aligned} \hat{P}_m (\partial_c \hat{H}) (\partial_a \hat{P}_n) \hat{P}_n = & (\partial_c E_m) \hat{P}_m (\partial_a \hat{P}_n) \hat{P}_n \\ & + E_m \hat{P}_m (\partial_c \hat{P}_m) (\partial_a \hat{P}_n) \hat{P}_n \\ & + \sum_{l \neq n,m} E_l \hat{P}_m (\partial_c \hat{P}_l) \hat{P}_l (\partial_a \hat{P}_n) \hat{P}_n \end{aligned} \quad (101)$$

and a similar expression for $\hat{P}_m (\partial_a \hat{H}) (\partial_c \hat{H}) \hat{P}_n$. We note that the summations over bands other than n and m cancel when combining all three contributions. We find

$$\begin{aligned} \text{tr}[(\partial_a \partial_c \hat{H}) + (\partial_c \hat{H}) (\partial_a \hat{P}_n) + (\partial_a \hat{P}_m) (\partial_c \hat{H})] \hat{P}_n (\partial_b \hat{P}_m) \hat{P}_m \\ = (\partial_a \epsilon_{nm}) Q_{cb}^{nm} + \epsilon_{nm} C_{a;bc}^{mn}, \end{aligned} \quad (102)$$

where we identified the two-state quantum geometric tensor Q_{bc}^{nm} and the two-state quantum geometric connection $C_{a;bc}^{mn}$ in combination with further spectral contributions. We recombine these spectral contributions with those obtained

previously defining

$$\mathfrak{s}_{nm}^{(1)}(\omega) \equiv \frac{i}{\gamma} \frac{(\partial_a \epsilon_{nm}) (\epsilon_{nm})^2 f_{nm}}{\omega + \epsilon_{nm} + i\Gamma}, \quad (103)$$

$$\mathfrak{s}_{nm}^{(2a)}(\omega) \equiv \frac{(\partial_a \epsilon_{nm}) \epsilon_{nm} f_{nm}}{\omega + \epsilon_{nm} + i\Gamma}, \quad (104)$$

$$\mathfrak{s}_{nm}^{(2b)}(\omega) \equiv \frac{(\epsilon_{nm})^2 f_{nm}}{\omega + \epsilon_{nm} + i\Gamma}, \quad (105)$$

which contains all dependencies on the band dispersions, the scattering rates, and driving frequency. We conclude by combining all previous results and obtain

$$\begin{aligned} \sigma^{a;bc}(\omega) = & \frac{e^3}{\hbar^2 \omega^2} \sum_{\substack{n,m \\ n \neq m}} \int_{\text{BZ}} (\mathfrak{s}_{nm}^{(1)}(\omega) Q_{cb}^{nm} + \mathfrak{s}_{nm}^{(1)}(-\omega) Q_{bc}^{nm}) \\ & - \frac{e^3}{\hbar^2 \omega^2} \sum_{\substack{n,m \\ n \neq m}} \int_{\text{BZ}} (\mathfrak{s}_{nm}^{(2a)}(\omega) Q_{cb}^{nm} + \mathfrak{s}_{nm}^{(2a)}(-\omega) Q_{bc}^{nm}) \\ & - \frac{e^3}{\hbar^2 \omega^2} \sum_{\substack{n,m \\ n \neq m}} \int_{\text{BZ}} (\mathfrak{s}_{nm}^{(2b)}(\omega) C_{a;bc}^{mn} + \mathfrak{s}_{nm}^{(2b)}(-\omega) C_{a;cb}^{mn}) \end{aligned} \quad (106)$$

in leading order in $\gamma/|\epsilon_{nm}| \ll 1$. We see the symmetry in $(c, \omega) \leftrightarrow (b, -\omega)$ as required by the definition given in Eq. (79). Focusing on the resonant parts via the replacement $[x + i\Gamma]^{-1} \rightarrow -i\pi \delta(x)$, we find that the second term in Eq. (106) vanishes. The first and third terms are identified as injection and shift current $\sigma^{a;bc}(\omega) = \sigma_{\text{inj}}^{a;bc}(\omega) + \sigma_{\text{shift}}^{a;bc}(\omega)$ given as

$$\sigma_{\text{inj}}^{a;bc}(\omega) \equiv \frac{2\pi e^3}{\gamma \hbar^2} \sum_{\substack{n,m \\ n \neq m}} \int_{\text{BZ}} \delta(\omega - \epsilon_{nm}) f_{nm} (\partial_a \epsilon_{nm}) Q_{bc}^{nm}, \quad (107)$$

$$\sigma_{\text{shift}}^{a;bc}(\omega) \equiv \frac{i\pi e^3}{\hbar^2} \sum_{\substack{n,m \\ n \neq m}} \int_{\text{BZ}} \delta(\omega - \epsilon_{nm}) f_{nm} (C_{a;cb}^{mn} - C_{a;bc}^{nm}). \quad (108)$$

These formulas agree with those given in Ref. [22], which we generalized to degenerate bands. The intraband relaxation rate γ within the two-lifetime model [25,51] corresponds to the relaxation time, at which the injection current eventually saturates [22,46]. For finite interband relaxation rate Γ , a third contribution is found in Eq. (106) as previously reported in Ref. [26]. Setting $\Gamma = 0$ in Eqs. (103) to (105) allows one to determine off-resonant contributions to the currents [52].

IV. CONCLUSION AND OUTLOOK

We have presented a general approach to handle the observable information encoded in the Bloch states of a crystalline material. The approach is built on projectors to represent the quantum states, which eliminates the gauge dependence. The advantage of the projector formalism is twofold. On the one hand, it offers a natural connection to a geometric description of the complex projective bundle that the Bloch states form. This quantum geometric description allows for a systematic identification of independent wave function properties [12,13] that serve as minimal

building blocks for physical observables. These minimal entities clarify connections between seemingly independent observables and point towards different phenomena. On the other hand, projector formalism simplifies the theoretical investigation of material properties and their response functions that crucially rely on the complex interplay of internal degrees of freedom, such as spin and atomic orbitals. In particular, topological and geometric insulators and metals that host highly complex quantum states, even in the noninteracting approximation, are included.

In the first part of this paper, we have introduced the basic concepts of the projector formalism and geometric description for Bloch states, called *quantum state geometry*. We closed this section by presenting the essential geometric invariants in the projector formalism involving the quantum metric, Berry curvatures, and their dipoles. We extended the set of geometric invariants beyond the quantum geometric tensor by introducing the corresponding two-state quantities and the quantum geometric connection, which capture quantum geometric properties such as skewness and torsion. We summarize these quantities in Table I. The presented formalism allows for a systematic construction of geometric invariants beyond those explicitly discussed, whose physical and geometric interpretations remain to be fully understood.

We provide two detailed applications of the formalism: the polarization distribution and the shift and injection current, which was the focus of the companion article [7]. Here, these examples serve as a guiding principle for future applications of formalism to other properties of crystalline materials. In particular, we anticipate that the strategy to identify the relevant geometric invariants for the second-order optical response functions generally simplifies derivations built on standard perturbation-theoretical approaches using Green's function methods, where projectors are naturally introduced via the Bloch Hamiltonian and the spectral representation of the Green's functions [15]. We note that the formalism for momentum-local observables, which is the main focus of this article, can be straightforwardly combined with a perturbative treatment of interaction [14], which requires the inclusion of global geometric invariants and, thus, suggests a rich platform for geometric effects beyond the quantum metric and Berry curvature.

ACKNOWLEDGMENTS

We thank A. Alexandradinata, O. Antebi, D. S. Borgnia, I. Esin, M. M. Hirschmann, T. Holder, F. de Juan, W. Jankowski, L. Šmejkal, M. Sonner, and T. V. Trevisan for stimulating discussions. A.A. was supported by a Kavli ENSI fellowship at UC Berkeley and the National Science Foundation (NSF) Convergence Accelerator Award No. 2235945 at MIT. J.M. was supported by the German National Academy of Sciences Leopoldina through Grant No. LPDS 2022-06 and, in part, by the Deutsche Forschungsgemeinschaft under Grant cluster of excellence ct.qmat (EXC 2147, Project No. 390858490). J.E.M. was supported by the Quantum Materials program under the Director, Office of Science, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, of the U.S. Department of Energy, Contract No. DE-AC02-05CH11231, at Lawrence Berkeley National Laboratory and a Simons Investigatorship.

APPENDIX A: EFFICIENT NUMERICAL EVALUATION OF PROJECTORS AND PROJECTOR DERIVATIVES

The numerical derivative requires diagonalizing the Hamiltonian at different momenta, where the obtained Bloch wave functions generically are not expressed in the same gauge. This arbitrary phase highly complicates a stable evaluation of the difference between the Bloch states, which is necessary for a numerical derivative. Explicit gauge fixing procedures are possible but tedious. In contrast, the projectors are gauge invariant by construction, so differences are directly well defined. The following describes the numerical steps required to obtain the geometric quantities presented in Sec. II and in the companion article [7].

1. Numerical projector construction

Consider a Bloch Hamiltonian $N_{\text{orb}} \times N_{\text{orb}}$ matrix $\hat{H}(\mathbf{k})$ for N_{orb} orbitals as a function of momentum $\mathbf{k}$. When diagonalized for a fixed momentum, we obtain the eigenvalues $E_n(\mathbf{k})$ and corresponding orthonormal eigenvectors $|u_n(\mathbf{k})\rangle$. For each index n , we construct a $N_{\text{orb}} \times N_{\text{orb}}$ matrix $\hat{P}_n(\mathbf{k})$ as tensor product between the eigenvector $|u_n\rangle$ and its complex transpose $\langle u_n|$, resulting in N_{orb} Hermitian matrices satisfying $\hat{P}_n \hat{P}_m = \delta_{nm} \hat{P}_m$ and $\hat{H} \hat{P}_n = E_n \hat{P}_n$ under ordinary matrix multiplication, thus satisfying Eqs. (3) to (5). If necessary, projectors onto degenerate or multiple bands are constructed by summing the respective $\hat{P}_n$. No specific gauge choice is required for $|u_n\rangle$ within this construction as long as $\langle u_n|$ is directly obtained from the corresponding $|u_n\rangle$ by complex transposition.

2. Numerical derivative construction

We denote the momentum unit vector in direction α as $\mathbf{e}_\alpha$. The first derivative of the projector is obtained by the symmetric finite difference,

$$\partial_\alpha \hat{P}_n(\mathbf{k}) = \frac{1}{2\lambda} [\hat{P}_n(\mathbf{k} + \lambda \mathbf{e}_\alpha) - \hat{P}_n(\mathbf{k} - \lambda \mathbf{e}_\alpha)] + O(\lambda^2), \quad (\text{A1})$$

with an error of order λ^2 . A complete set of projector derivatives in d spatial dimensions requires $2d$ diagonalizations of the Hamiltonian for each momentum $\mathbf{k}$. The second derivative is obtained by

$$\partial_\alpha \partial_\alpha \hat{P}_n(\mathbf{k}) = \frac{1}{\lambda^2} [\hat{P}_n(\mathbf{k} + \lambda \mathbf{e}_\alpha) - 2\hat{P}_n(\mathbf{k}) + \hat{P}_n(\mathbf{k} - \lambda \mathbf{e}_\alpha)] + O(\lambda^2). \quad (\text{A2})$$

A complete set of second-order derivatives requires one further diagonalization of the Hamiltonian. For the off-diagonal second-order derivative, we use

$$\begin{aligned} \partial_\alpha \partial_\beta \hat{P}_n(\mathbf{k}) = & \frac{1}{2\lambda^2} [\hat{P}_n(\mathbf{k} + \lambda [\mathbf{e}_\alpha + \mathbf{e}_\beta]) \\ & - \hat{P}_n(\mathbf{k} + \lambda \mathbf{e}_\alpha) - \hat{P}_n(\mathbf{k} + \lambda \mathbf{e}_\beta) + 2\hat{P}_n(\mathbf{k}) \\ & - \hat{P}_n(\mathbf{k} - \lambda \mathbf{e}_\alpha) - \hat{P}_n(\mathbf{k} - \lambda \mathbf{e}_\beta) \\ & + \hat{P}_n(\mathbf{k} - \lambda [\mathbf{e}_\alpha + \mathbf{e}_\beta])] + O(\lambda^2), \end{aligned} \quad (\text{A3})$$

which requires $d(d-1)$ further diagonalizations due to the $\mathbf{e}_\alpha + \mathbf{e}_\beta$ directions. In total, $2d + 1 + d(d-1) = 1 + d + d^2$ diagonalizations are required to obtain a complete set of first- and second-order derivatives in d dimensions, that is, 3 for one, 7 for two, and 13 for three dimensions. These numbers can be reduced, for instance, when focusing only on one spatial direction. A λ of size 10^{-3} to 10^{-5} is usually sufficient for stable and reliable numerical results. The numerical accuracy can be checked by various projector identities such as Eqs. (50) to (52).

APPENDIX B: STRATEGY TO DETERMINE CLOSED ANALYTIC FORMS FOR FEW-BAND SYSTEMS

We describe how to relate the results of Ref. [8] to the presented formalism. Let us consider the generators $\hat{M}_\alpha$ of $SU(N)$ and expand the Bloch Hamiltonian,

$$\hat{H} = h_0 \mathbb{1}_N + \sum_{\alpha} h_{\alpha} \hat{M}_{\alpha}, \quad (\text{B1})$$

where we have defined h_0 related to the trace of the Hamiltonian and h_{α} as the coefficient of the generator expansion for the traceless part. For a two-band model, such an expansion is given by the well-known form $\hat{H} = d_0 \mathbb{1}_2 + \mathbf{d} \cdot \boldsymbol{\sigma}$ with Pauli matrices $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. Similarly, we expand the projector onto the band eigenstates as

$$\hat{P}_n = \frac{r}{N} \mathbb{1}_N + \sum_{\alpha} P_{n\alpha} \hat{M}_{\alpha}, \quad (\text{B2})$$

where r is the rank of the projector and $P_{n\alpha}$ the expansion coefficient for a given band index n and generator α . As an example, the two projectors for a two-band model take the well-known form $\hat{P}_{\pm} = \frac{1}{2}(\mathbb{1}_2 \pm \mathbf{n} \cdot \boldsymbol{\sigma})$ with $\mathbf{n} = \mathbf{d}/|\mathbf{d}|$. The gauge-invariant matrix elements $M_{\alpha}^{nm} = \langle u_n | \hat{M}_{\alpha} | u_m \rangle$ introduced in Ref. [8] are related to the projector coefficients via

$$M_{\alpha}^{nm} \equiv \langle u_n | \hat{M}_{\alpha} | u_n \rangle = \text{tr}[\hat{M}_{\alpha} \hat{P}_n] = 2P_{n\alpha} \quad (\text{B3})$$

using $\text{tr}[\hat{M}_{\alpha} \hat{M}_{\beta}] = 2\delta_{\alpha\beta}$. Higher-order generators are obtained analogously; for instance,

$$\begin{aligned} M_{\alpha}^{nm} M_{\beta}^{mn} &\equiv \langle u_n | \hat{M}_{\alpha} | u_m \rangle \langle u_m | \hat{M}_{\beta} | u_n \rangle \\ &= \text{tr}[\hat{P}_n \hat{M}_{\alpha} \hat{P}_m \hat{M}_{\beta}] \\ &= \sum_{\mu, \nu} P_{n\mu} P_{m\nu} \text{tr}[\hat{M}_{\mu} \hat{M}_{\alpha} \hat{M}_{\nu} \hat{M}_{\beta}], \end{aligned} \quad (\text{B4})$$

where we can evaluate the trace explicitly via the defining equation of the $SU(N)$ algebra, $\hat{M}_{\alpha} \hat{M}_{\beta} = 2/N \delta_{\alpha\beta} \mathbb{1}_N + \sum_{\gamma} S_{\alpha\beta\gamma} \hat{M}_{\gamma}$ with complex structure factors $S_{\alpha\beta\gamma} = d_{\alpha\beta\gamma} + if_{\alpha\beta\gamma}$, capturing the anticommutation and commutation relations as real and imaginary parts, respectively [8]. We obtain

$$M_{\alpha}^{nm} M_{\beta}^{mn} = \frac{4}{N} P_{n\alpha} P_{m\beta} + 2 \sum_{\mu, \nu, \gamma} S_{\mu\alpha\gamma} S_{\nu\beta\gamma} P_{n\mu} P_{m\nu}. \quad (\text{B5})$$

As long as only gauge-invariant combinations of matrix elements are considered, they can be expressed in terms of the projectors, which we presented as our building block for the geometric description. The geometric objects presented in

the main text can be evaluated by inserting Eq. (B2) and using the $SU(N)$ algebra to evaluate the trace of generators.

APPENDIX C: QUANTUM GEOMETRIC QUANTITIES FOR NONDEGENERATE BANDS

We present the quantum geometric invariants introduced in Sec. II F in terms of the Bloch states $|u_n\rangle$ of a nondegenerate band to provide the connections to the existing forms of the geometric invariants in the literature. The band projector of interest reads $\hat{P}_n = |u_n\rangle\langle u_n|$ in this case.

1. Quantum geometric tensor

Expressed in terms of Bloch states, the quantum geometric tensor in Eq. (16) takes the familiar form

$$Q_{\alpha\beta}^n = \langle \partial_{\alpha} u_n | \partial_{\beta} u_n \rangle + \langle u_n | \partial_{\alpha} u_n \rangle \langle u_n | \partial_{\beta} u_n \rangle, \quad (\text{C1})$$

from which the quantum metric and Berry curvature expressed in Bloch states is straightforwardly derived. In order to derive the two-state quantum geometric tensor in terms of Bloch states we first obtain

$$\hat{\mathcal{E}}_{\alpha}^{mn} = i \hat{P}_m \partial_{\alpha} \hat{P}_n \hat{P}_m = (1 - \delta_{mn}) r_{mn}^{\alpha} |u_m\rangle\langle u_n|, \quad (\text{C2})$$

involving the non-Abelian Berry connection $r_{mn}^{\alpha} = i \langle u_m | \partial_{\alpha} u_n \rangle = -i \langle \partial_{\alpha} u_m | u_n \rangle$. The quantity (C2) was introduced in Ref. [23] as tangent basis vectors for $U(N)/U(1)^N$ and related to transition dipole matrix elements. Using this identity and focusing on $n \neq m$ for Eq. (20) only, we see

$$Q_{\alpha\beta}^{mn} = -\text{tr}[\hat{\mathcal{E}}_{\alpha}^{mn} \hat{\mathcal{E}}_{\beta}^{mn}] \quad (\text{C3})$$

$$= -(1 - \delta_{nm})^2 r_{nm}^{\alpha} r_{mn}^{\beta} \text{tr}[|u_n\rangle\langle u_m| u_m\rangle\langle u_n|] \quad (\text{C4})$$

$$= -(1 - \delta_{nm}) r_{nm}^{\alpha} r_{mn}^{\beta}, \quad (\text{C5})$$

which establishes the connection between the product of the non-Abelian Berry connections and the two-state quantum geometric tensor.

2. Quantum geometric connection

Inserting the explicit form of band projector onto a nondegenerate band into Eq. (27), we obtain

$$\begin{aligned} Q_{\alpha;\beta\gamma}^n &= \frac{1}{2} \langle \partial_{\alpha} u_n | \partial_{\beta} \partial_{\gamma} u_n \rangle + \frac{1}{2} \langle u_n | \partial_{\alpha} u_n \rangle \langle u_n | \partial_{\beta} \partial_{\gamma} u_n \rangle \\ &\quad - \langle \partial_{\alpha} u_n | \partial_{\beta} u_n \rangle \langle u_n | \partial_{\gamma} u_n \rangle \\ &\quad - \langle u_n | \partial_{\alpha} u_n \rangle \langle u_n | \partial_{\beta} u_n \rangle \langle u_n | \partial_{\gamma} u_n \rangle + (\beta \leftrightarrow \gamma). \end{aligned} \quad (\text{C6})$$

The expression shows explicitly that the projector form yields a much compacter form even for nondegenerate bands. In order to derive the explicit form of the two-state quantum geometric connection given in Eq. (31) for $n \neq m$, we use Eq. (C2) and obtain

$$C_{\alpha;\beta\gamma}^{mn} = -\text{tr}[\hat{\mathcal{E}}_{\beta}^{nm} \partial_{\alpha} \hat{\mathcal{E}}_{\gamma}^{mn}] \quad (\text{C7})$$

$$= -(1 - \delta_{nm})^2 r_{nm}^{\beta} \text{tr}[|u_n\rangle\langle u_m| \partial_{\alpha} (r_{mn}^{\gamma} |u_m\rangle\langle u_n|)] \quad (\text{C8})$$

$$= -(1 - \delta_{nm}) r_{nm}^{\beta} (\partial_{\alpha} r_{mn}^{\gamma} - i(\xi_m^{\alpha} - \xi_n^{\alpha}) r_{mn}^{\gamma}) \quad (\text{C9})$$

$$= -(1 - \delta_{nm}) r_{nm}^{\beta} r_{mn;\alpha}^{\gamma}, \quad (\text{C10})$$

with band Berry connection $\xi_n^\alpha = r_{nm}^\alpha = i\langle u_n | \partial_\alpha u_n \rangle$ and covariant derivative of the non-Abelian Berry connection, $r_{mn;a}^\gamma = \partial_\alpha r_{mn}^\gamma - i(\xi_m^\alpha - \xi_n^\alpha) r_{mn}^\gamma$.

3. Interband Wilson loop and shift vector

We derive the explicit expression for the interband Wilson loop in Eq. (37) for nondegenerate bands using Eq. (C2). We obtain

$$W_{\alpha\beta}^{mn}(\mathbf{k}, \mathbf{q}) = \text{tr}[\hat{e}_\beta^{nm}(\mathbf{k}) \hat{e}_\alpha^{mn}(\mathbf{k} + \mathbf{q})] \quad (\text{C11})$$

$$= (1 - \delta_{nm}) r_{nm}^\beta(\mathbf{k}) r_{mn}^\alpha(\mathbf{k} + \mathbf{q}) \times \text{tr}[|u_n(\mathbf{k})\rangle \langle u_n(\mathbf{k})| u_m(\mathbf{k} + \mathbf{q})\rangle \langle u_m(\mathbf{k} + \mathbf{q})|] \quad (\text{C12})$$

$$= (1 - \delta_{nm}) r_{mn}^\alpha(\mathbf{k} + \mathbf{q}) r_{nm}^\beta(\mathbf{k}) \times \langle u_n(\mathbf{k}) | u_m(\mathbf{k} + \mathbf{q}) \rangle \langle u_n(\mathbf{k} + \mathbf{q}) | u_n(\mathbf{k}) \rangle, \quad (\text{C13})$$

where we recover the expression given in Ref. [44] with explicitly subtracted intraband contribution $n = m$. Using the definition of the shift vector in Eq. (39) and inserting the expressions for the two-state quantum geometric tensor and quantum geometric connection given in Eqs. (C5) and (C10) gives

$$R_{\alpha\beta}^{mn} = i \frac{C_{\alpha;\beta\beta}^{mn}}{Q_{\beta\beta}^{mn}} = i \frac{r_{nm}^\beta r_{mn;\alpha}^\beta}{r_{nm}^\beta r_{mn}^\beta} = i \frac{r_{mn;\alpha}^\beta}{r_{mn}^\beta} \quad (\text{C14})$$

$$= i \frac{\partial_\alpha r_{mn}^\beta - i(\xi_m^\alpha - \xi_n^\alpha) r_{mn}^\beta}{r_{mn}^\beta} \quad (\text{C15})$$

$$= \xi_m^\alpha - \xi_n^\alpha + i \partial_\alpha \ln r_{mn}^\beta. \quad (\text{C16})$$

We recover the standard definition of the shift current [23,46] in terms of the band Berry connection $\xi_n^\alpha = r_{nm}^\alpha = i\langle u_n | \partial_\alpha u_n \rangle$ and the non-Abelian Berry connection $r_{mn}^\alpha = i\langle u_m | \partial_\alpha u_n \rangle$.

APPENDIX D: DERIVATION OF THE GENERATING FUNCTION OF THE POLARIZATION DISTRIBUTION

We provide the derivation from Eq. (73) to (74), which follows the steps presented first in Ref. [12] by one of us. We note the identity

$$C(\mathbf{q}) + C(\mathbf{q}') = \int_{\text{BZ}} \log \det(\langle u_i(\mathbf{k}) | \hat{P}_{\mathbf{k}+\mathbf{q}} | u_j(\mathbf{k} + \mathbf{q} + \mathbf{q}') \rangle)_{ij}, \quad (\text{D1})$$

where $\hat{P}_{\mathbf{k}} = \sum_{n \in \text{occ}} |u_n(\mathbf{k})\rangle \langle u_n(\mathbf{k})|$ is the projector onto all occupied bands. Using this, we obtain

$$\log C(-\mathbf{q} - \mathbf{q}') + \log C(\mathbf{q}) + \log C(\mathbf{q}') = \int_{\text{BZ}} \log \det_{i_k} [\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{q}} \hat{P}_{\mathbf{k}+\mathbf{q}+\mathbf{q}'} \hat{P}_{\mathbf{k}}]. \quad (\text{D2})$$

We note that

$$\log[C(\mathbf{q})C(-\mathbf{q})] = \int_{\text{BZ}} \log \det_{i_k} [\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{q}} \hat{P}_{\mathbf{k}}], \quad (\text{D3})$$

so that we arrive at

$$\log \frac{C(\mathbf{q} + \mathbf{q}')}{C(\mathbf{q})C(\mathbf{q}')} = - \int_{\text{BZ}} \log \det_{i_k} [\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{q}} \hat{P}_{\mathbf{k}+\mathbf{q}+\mathbf{q}'} \hat{P}_{\mathbf{k}}] + \int_{\text{BZ}} \log \det_{i_k} [\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{q}+\mathbf{q}'} \hat{P}_{\mathbf{k}}]. \quad (\text{D4})$$

It is convenient to define $b_{\mathbf{v}}(t) = \log C(\mathbf{v}t)$, for which we obtain

$$\begin{aligned} \partial_t b_{\mathbf{v}}(t) - \partial_t b_{\mathbf{v}}(0) &= - \int_{\text{BZ}} \text{tr}[(\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{v}t} \hat{P}_{\mathbf{k}})^{-1} \hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{v}t} (\partial_t \hat{P}_{\mathbf{k}+\mathbf{v}t}) \hat{P}_{\mathbf{k}}] \\ &\quad + \int_{\text{BZ}} \text{tr}[(\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{v}t} \hat{P}_{\mathbf{k}})^{-1} \hat{P}_{\mathbf{k}} (\partial_t \hat{P}_{\mathbf{k}+\mathbf{v}t}) \hat{P}_{\mathbf{k}}] \end{aligned} \quad (\text{D5})$$

via Jacobi's formula

$$\frac{d}{dt} \det A(t) = \det[A(t)] \text{tr} \left[A^{-1}(t) \frac{d}{dt} A(t) \right]. \quad (\text{D6})$$

Both terms in Eq. (D5) can be combined via the projector identity $\partial_t \hat{P}_t = (\partial_t \hat{P}_t) \hat{P}_t + \hat{P}_t (\partial_t \hat{P}_t)$, such that we identify

$$\mathcal{A}_{\alpha}^{\mathbf{k}}(\mathbf{k}') = \text{tr}[\hat{P}_{\mathbf{k}} (\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}'} \hat{P}_{\mathbf{k}})^{-1} \hat{P}_{\mathbf{k}} (\partial_\alpha \hat{P}_{\mathbf{k}'} \hat{P}_{\mathbf{k}})]. \quad (\text{D7})$$

With that, we write

$$\partial_t b_{\mathbf{v}}(t) - \partial_t b_{\mathbf{v}}(0) = \sum_{\alpha} \mathbf{e}_{\alpha} \mathcal{A}_{\alpha}^{\mathbf{k}}(\mathbf{k} + \mathbf{v}t), \quad (\text{D8})$$

where $\mathbf{e}_{\alpha}$ is the unit vector in the direction of $\mathbf{v}$. Integrating this equation, we arrive at Eq. (74), where the constant $\mathcal{A}_{\alpha} = \sum_{n \in \text{occ}} \int_{\text{BZ}} \mathcal{A}_{\alpha}^n(\mathbf{k})$ is fixed by the known relation between the mean polarization and the Berry connection.

APPENDIX E: DERIVATION OF THE TWO REMAINING CONTRIBUTIONS TO THE INJECTION AND SHIFT CURRENT

1. Vanishing of the contribution $\sigma_{(0)}^{a;bc}$

We show that $\sigma_{(0)}^{a;bc}$ defined as

$$\sigma_{(0)}^{a;bc} = \text{tr} \left[\hat{P}_{\text{occ}} \left(\partial_a \partial_b \partial_c \hat{H} + \left[\partial_b \partial_c \hat{H}, \frac{\partial_a \hat{H}}{-\epsilon + i\gamma} \right] \right) \right] \quad (\text{E1})$$

vanishes in leading orders of $\gamma \ll |\epsilon_{nm}|$. Using the separation of the fraction into two contributions as given in Eq. (85), we see that insertion of the first term leads to a vanishing contribution via Eq. (87),

$$-\frac{i}{\gamma} \sum_n (\partial_a E_n) \text{tr}[\hat{P}_{\text{occ}} [\partial_b \partial_c \hat{H}, \hat{P}_n]] = 0. \quad (\text{E2})$$

Inserting the second term to leading order in $\gamma \ll |\epsilon_{nm}|$ reads

$$\sum_n \text{tr}[\hat{P}_{\text{occ}} [\partial_b \partial_c \hat{H}, (\partial_a \hat{P}_n) \hat{P}_n]]. \quad (\text{E3})$$

Inserting the explicit form of $\hat{P}_{\text{occ}}$ given in Eq. (82) and using the derivative identity $\hat{P}_n (\partial_a \hat{P}_n) = \delta_{nm} \partial_a \hat{P}_n - (\partial_a \hat{P}_n) \hat{P}_m$

leads to

$$\sum_{n,m} f_m \text{tr}[(\partial_a \hat{P}_n) \hat{P}_m (\partial_b \partial_c \hat{H}) - \hat{P}_m (\partial_a \hat{P}_n) \hat{P}_n (\partial_b \partial_c \hat{H})] \\ = \sum_{n,m} f_m \text{tr}[(\partial_a \hat{P}_m) \hat{P}_n (\partial_b \partial_c \hat{H})] \quad (\text{E4})$$

$$= \sum_n f_n \text{tr}[(\partial_a \hat{P}_n) (\partial_b \partial_c \hat{H})]. \quad (\text{E5})$$

We performed the sum $\sum_n \hat{P}_n = \hat{1}$ in the last step. We see that the result is equal to the $-\text{tr}[\hat{P}_{\text{occ}} (\partial_a \partial_b \partial_c \hat{H})]$ under the momentum integral assuming a momentum constant f_n and performing a partial integration in the a direction, so that $\sigma_{(0)}^{abc}$ vanishes.

2. Leading-order contributions to $\sigma_{(1)}^{abc}(\omega)$

We evaluate the remaining contribution to Eq. (80), which takes the form $\sigma_{(1)}^{abc}(\omega) = A^{b,ac}(\omega) + A^{c,ab}(-\omega)$

with

$$A^{a,bc}(\omega) \equiv \text{tr} \left[\hat{P}_{\text{occ}} \left[\frac{\partial_a \hat{H}}{\omega + \epsilon + i\Gamma}, \partial_b \partial_c \hat{H} \right] \right]. \quad (\text{E6})$$

We decompose the fraction via Eq. (84). The first term leads to

$$\text{tr}[\hat{P}_{\text{occ}} [\hat{P}_n, \partial_b \partial_c \hat{H}]] = 0, \quad (\text{E7})$$

which vanishes due to identity (87). The second term involves

$$\text{tr}[\hat{P}_{\text{occ}} [\hat{P}_n (\partial_a \hat{P}_m) \hat{P}_m, \partial_b \partial_c \hat{H}]] \quad (\text{E8})$$

$$= f_{nm} \text{tr}[(\partial_b \partial_c \hat{H}) \hat{P}_n (\partial_a \hat{P}_m) \hat{P}_m], \quad (\text{E9})$$

which we simplified via identity (88). Determining the prefactors and combining the contributions leads to the form given in Eq. (99).

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