

Multistate Geometry of Shift Current and Polarization

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The quantum metric and Berry curvature capture essential properties of nontrivial Bloch states and underpin many fascinating phenomena. However, it becomes increasingly evident that a more comprehensive understanding of quantum state geometry is necessary to explain properties involving Bloch states of multiple bands, such as optical transitions. To this end, we employ quantum state projectors to develop an explicitly gauge-invariant formalism and demonstrate its power with applications to nonlinear optics and the theory of electronic polarization. We provide a simple expression for the shift current that resolves its precise relation to the moments of electronic polarization, clarifies the treatment of band degeneracies, and reveals its decomposition into the sum of the skewness of the occupied states and intrinsically multistate geometry. The projector approach is applied to calculate nonlinear optical properties of transition metal dichalcogenides (TMDs) layers, using previously calculated minimal tight-binding models, and demonstrated analytically on a three-band generalization of the Rice-Mele chain to elucidate the different contributions. We close with comments on further applications of the projector operator approach to multistate geometry.

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Introduction—The presence of a crystal lattice with multiple orbitals per unit cell not only leads to (potentially degenerate) band dispersions $E_n(\mathbf{k})$ but also, in general, to a nontrivial evolution with crystal momentum $\mathbf{k}$ of the Bloch states, which captures the spatially periodic part of the lattice eigenstates. The implications of evolving Bloch states have been extensively studied in the emerging field of quantum state geometry, which aims to describe Bloch state properties and their observable consequences using the Berry phase and curvature [1–3], among other lesser-known quantities. In particular, the quantum metric of Bloch states has attracted much attention in recent years as relevant, for example, for superconductivity [4–6] and normal-state transport [7–10] in flat-band materials, the capacitance of insulators [11], and fractional Chern insulator physics [12–14].

The existence and importance of geometrical properties beyond the Berry curvature and quantum metric have also become evident. Besides various generalizations [15–19],

efforts toward a comprehensive geometric analysis of the Bloch state manifold have revealed new independent geometric quantities involving additional momentum derivatives, multiple momenta, and several band states [20–25], whose consequences for even uncorrelated electrons in multiorbital systems are far from completely understood. Linear and nonlinear optical responses are natural candidates for the physical manifestation of multistate quantum geometry due to their momentum-local coupling of the Bloch states of multiple bands [21,26–28]. Whereas first-order optical responses only couple to the two-state quantum metric and Berry curvature [29], second- and higher-order optical responses involve higher-order tensors [20,21,30–32] implying geometrical optical sum rules and other results [19,29,32–36]. Multiple-band properties require new concepts of multistate geometry beyond the broadly studied geometry of single bands or even adiabatic multiband properties like the magnetoelectric effect [37–39]. The shift current is an example of the implications of band geometry for technology as it forms one piece of the bulk photovoltaic effect in noncentrosymmetric materials [28,40–43]. Hence, a comprehensive understanding of the geometry of optical responses would help guide their identification and their realization in materials.

In this Letter, we develop a general approach to computing the geometrical properties of Bloch states, which we apply to shift current and the polarization distribution. Our approach starts from the Bloch

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Hamiltonian that determines both band dispersions and Bloch states,

$$\hat{H}(\mathbf{k}) = \sum_{n \in \text{bands}} E_n(\mathbf{k}) \hat{P}_n(\mathbf{k}), \quad (1)$$

where we conveniently express the band Bloch states in a gauge-invariant form via orthogonal projectors $\hat{P}_n(\mathbf{k})$ fulfilling $\hat{P}_n(\mathbf{k})\hat{P}_m(\mathbf{k}) = \delta_{nm}\hat{P}_n(\mathbf{k})$ [13,16,23–25,44,45]. The formalism developed in terms of these projection operators enables us to clarify the relation between the shift current and the polarization and unify sum rules in previous special cases [27,28,46,47]. It also solves challenges in the treatment of degenerate bands [26], which we combine with a complete geometric characterization of the polarization of a generic band insulator. Generalizing previous single-band results [23,29], we identify the geometry associated with the Slater determinant ground state of uncorrelated electron systems, presenting Plücker embedding (essentially a formalization of Slater determinants) as a convenient description for degenerate subspaces [24]. An advantage of the formulas based on projectors is their explicit gauge invariance, and we apply full and simplified versions of the resulting expressions for optical properties to three-band models of transition metal dichalcogenides (TMDs) [48] to demonstrate their practical utility. In the companion work [49], we complement the physical insights with considerably more technical details on the projector formalism and the geometrical invariants focusing on broadly relevant algebraic relationships and detailed example calculations.

Geometry of shift current—The DC components of the second-order optical response under uniform illumination

$$j^\alpha(0) = \sum_{\beta,\gamma} \left(\sigma_{\text{inj}}^{\alpha;\beta\gamma}(\omega) + \sigma_{\text{shift}}^{\alpha;\beta\gamma}(\omega) \right) \mathcal{E}^\beta(\omega) \mathcal{E}^\gamma(-\omega) \quad (2)$$

decomposes into the injection and shift current with Fourier components of the electric fields $\mathcal{E}^\beta(\omega)$ [20,21,26,30,31]. The injection current involves the two-state (second-order) quantum geometric tensor $Q_{\beta\gamma}^{mn}$ [20], whereas the shift current is determined by the two-state third-order quantum geometric connection $C_{\alpha;\beta\gamma}^{mn}$ [20,21], whose symmetric and antisymmetric components determine the linear and circular shift current [50] via

$$\sigma_{\text{shift}}^{\alpha;(\beta\gamma)}(\omega) = -\frac{2\pi e^3}{\hbar^2} \sum_{n,m} \int_{\mathbf{k}} \delta(\omega - \epsilon_{mn}) f_{nm} \text{Im} C_{\alpha;(\beta\gamma)}^{[mn]}, \quad (3)$$

$$\sigma_{\text{shift}}^{\alpha;[\beta\gamma]}(\omega) = -\frac{2i\pi e^3}{\hbar^2} \sum_{n,m} \int_{\mathbf{k}} \delta(\omega - \epsilon_{mn}) f_{nm} \text{Re} C_{\alpha;[\beta\gamma]}^{(mn)}, \quad (4)$$

where we indicate (anti)symmetrization in the indices as $(\beta\gamma)$ and $[\beta\gamma]$. We assumed $\omega > 0$ and bands sorted by

increasing energy. $\epsilon_{nm} \equiv E_n - E_m$ and $f_{nm} = f_n - f_m$ denote the band gaps and Fermi function differences. We omit the momentum dependence for brevity. The momentum integral reads $\int_{\mathbf{k}} \equiv \int_{\text{BZ}} d^d \mathbf{k} / (2\pi)^d$ in d dimensions and the electron's charge is $-e$ with $e > 0$.

Multistate geometry—The second- and third-order geometric tensors $Q_{\beta\gamma}^{mn}$ and $C_{\alpha;\beta\gamma}^{mn}$ in projector form read,

$$Q_{\beta\gamma}^{mn} \equiv \text{tr} \left[\hat{P}_n (\partial_\beta \hat{P}_m) (\partial_\gamma \hat{P}_n) \right], \quad (5)$$

$$C_{\alpha;\beta\gamma}^{mn} \equiv \text{tr} \left[\hat{P}_n (\partial_\beta \hat{P}_m) [(\partial_\alpha \partial_\gamma \hat{P}_n) + (\partial_\alpha \hat{P}_m) (\partial_\gamma \hat{P}_n)] \right], \quad (6)$$

with momentum derivatives $\partial_\alpha \equiv \partial_{k_\alpha}$. The diagonal component of $Q_{\beta\gamma}^{nn} = g_{\beta\gamma}^n - (i/2)\Omega_{\beta\gamma}^n$ yields the quantum metric and Berry curvature of band n as real and imaginary part. The single-band component of $C_{\alpha;\beta\gamma}^{nn} = \text{tr} [\hat{P}_n (\partial_\beta \hat{P}_n) (\partial_\alpha \partial_\gamma \hat{P}_n)]$ is a novel independent extrinsic geometric quantity of band n [23]. The two terms in Eq. (6) are different from the separation used to clarify the real-space and momentum-space parts of the shift vector [53] as both terms are separately gauge invariant.

A key reason to write the geometric objects in the form of Eqs. (5) and (6) is that they generalize naturally from two states to two subspaces: replacing single-band projectors by subspace projectors, e.g., double-degenerate bands $\hat{P}_n = \hat{P}_{(n1)} + \hat{P}_{(n2)}$ or $\hat{P}_{\text{occ}} = \sum_{n \in \text{occ}} \hat{P}_n$ for the subspace of occupied bands; the $\otimes_n U(N_n)$ -gauge invariance under unitary transformations of the N_n -degenerate subspaces is evident in this formalism by gauge-invariance of each projector. The gauge invariance shortens analytic expressions, removing unphysical redundancies, and allows for a straightforward numerical evaluation [49] as the projectors can be chosen to be smooth over the whole Brillouin zone away from band crossings, unlike the Bloch states [16].

In previous derivations of the injection and shift currents [20,21,26], the treatment of degenerate bands remained challenging. In Ref. [26], degeneracies of the symmetric contribution $\sigma_{\text{shift}}^{\alpha;(\beta\gamma)}$ were treated in the basis where degenerate bands are split according to $\sum_\alpha \mathcal{E}^\alpha \langle u_{(ns)} | \partial_\alpha u_{(nl)} \rangle = 0$ for $s \neq l$, where s, l label different Bloch states $|u_{(ns)}\rangle$ within the degenerate band n . More recently, gauge invariance was assured by summing over the degenerate subspace explicitly [20,21]. The projector formulation in Eqs. (5) and (6) suggests a treatment of degenerate and nondegenerate bands on an equal footing by only adjusting the corresponding band projectors. Indeed, we show by explicit calculation presented in the companion paper [49] that the derivation of Eq. (2) only requires the Hamiltonian decomposition given in Eq. (1), where the projectors $\hat{P}_n = \sum_{s=1}^{N_n} \hat{P}_{(ns)}$ may project onto N_n -degenerate band subspaces. We note that finite intra- and interband relaxation rates [30] enable further contributions to the shift

current [31,49] and allow the inclusion of effectively degenerate bands [16].

While the separation of the two-state quantum metric and Berry curvature as symmetric and antisymmetric parts of $Q_{\beta\gamma}^{mn}$ is well established, the quantum geometric connection yields a more complex structure, revealed by symmetrization of the band and external indices [50],

$$C_{\alpha;\beta\gamma}^{mn} = \frac{1}{2} \partial_\alpha Q_{\beta\gamma}^{mn} + \text{Re} C_{\alpha;[\beta\gamma]}^{(mn)} + i \text{Im} C_{\alpha;(\beta\gamma)}^{[mn]}, \quad (7)$$

for $n \neq m$. Note the connection between the symmetry in the band indices and being purely real and imaginary. Interestingly, given as the first term, the quantum metric and Berry curvature dipole [54,55] are part of the tensor. The linear and circular shift currents provide the remaining information about $C_{\alpha;\beta\gamma}^{mn}$.

The shift current can be related to a generalized Wilson loop associated with interband transitions at separated momenta [28,56,57]. This description is expressible in the projector approach by defining the interband Wilson loop as $W_{\alpha\beta}^{mn}(\mathbf{k}, \mathbf{q}) = \text{tr}[\hat{e}_\beta^{nm}(\mathbf{k}) \hat{e}_\alpha^{mn}(\mathbf{k} + \mathbf{q})]$ with the gauge-invariant interband dipole moments in projector form $\hat{e}_\alpha^{mn} = i \hat{P}_m (\partial_\alpha \hat{P}_m) \hat{P}_m$ [21,49]. The Wilson loop representation of the shift vector [57] leads to the projector form $R_{\alpha\beta}^{mn}(\mathbf{k}) = i C_{\alpha;\beta\gamma}^{mn}(\mathbf{k}) / Q_{\beta\gamma}^{mn}(\mathbf{k})$, which reduces to the conventional definition [21,26] for nondegenerate bands [49].

Geometric sum rules—Equation (3) and (4) imply that the linear and the circular shift current are, after frequency integration, entirely independent of band energies for an insulator and, thus, purely geometric. Therefore, they resemble the well-known Souza-Wilkens-Martin sum rule, which relates the optical conductivity to the integrated quantum metric of the occupied states interpreted as the ground state spread in real space [29].

One might wonder whether it is possible to generally reduce $C_{\alpha;\beta\gamma}^{mn}$ to the projector $\hat{P}_{\text{occ}}$ on all occupied bands upon band summation. Surprisingly, this is not possible for systems with more than two bands. As an illustration, we consider a single (potentially degenerate) filled band $\hat{P}_{\text{occ}} = \hat{P}_0$. The summation of the unoccupied subspace leads to

$$\begin{aligned} \sum_{m \in \text{unocc}} C_{\alpha;\beta\gamma}^{m0} = & -\text{tr}[\hat{P}_{\text{occ}} (\partial_\beta \hat{P}_{\text{occ}}) (\partial_\alpha \partial_\gamma \hat{P}_{\text{occ}})] \\ & + \text{tr} \left[\hat{P}_{\text{occ}} \left(\sum_{m \in \text{unocc}} (\partial_\beta \hat{P}_m) (\partial_\alpha \hat{P}_m) \right) (\partial_\gamma \hat{P}_{\text{occ}}) \right], \end{aligned} \quad (8)$$

where the generically nonzero second term involves the sum over all unoccupied bands. Further terms arise when the occupied subspace involves multiple bands at different energies [50]. Thus, the shift current sum rule does not

reduce to a ground state property of the occupied subspace, unlike the Souza-Wilkens-Martin sum rule [29].

We can relate part of the deviation from a ground state property to the torsion tensor, a purely two-state geometric quantity. Building on the previous definition [21,32], we express torsion in terms of the two subspace projectors $\hat{P}_n$ and $\hat{P}_m$,

$$T_{\beta;\alpha\gamma}^{mn} = \text{tr}[\hat{P}_n (\partial_\beta \hat{P}_m) (\partial_\alpha \hat{P}_m) (\partial_\gamma \hat{P}_n)] - (\alpha \leftrightarrow \gamma). \quad (9)$$

It is symmetric in its last two indices and vanishes for $n = m$ [50]. The symmetrized sum rule of the circular shift current in Eq. (4) relates to the real part of the momentum-integrated and band-traced torsion via the second term in Eq. (8) [32,50] and is quantized in some real-valued three- and four-band models [32,58]. We expect further purely multistate geometric quantities to be essential for higher-order optical responses, which remain to be identified and characterized.

Polarization distribution—We take a closer look at the first term in Eq. (8) and establish its relationship to the modern theory of polarization [59,60]. The primary tool in this construction is the reduction of the geometry of the occupied bands captured by $\hat{P}_{\text{occ}}$ to the geometry of a single state $|\Psi\rangle$ via the Plücker embedding, whose details we carefully discuss in the companion paper [49]. For this, we consider the polarization operator of all electrons $\hat{\mathbf{P}} = -e \hat{\mathbf{X}}$ involving the many-body position operator $\hat{\mathbf{X}} = \sum_{i \in \text{sites}} \hat{\mathbf{x}}_i$. The generating function of its moments reads

$$C(\mathbf{q}) = \langle \Psi | e^{i\mathbf{q} \cdot \hat{\mathbf{X}}} | \Psi \rangle \quad (10)$$

concerning the ground state wave function $|\Psi\rangle$. Assuming that $|\Psi\rangle$ is a Slater determinant constructed out of occupied bands, we obtain a closed formula for all cumulants of the distribution [49]

$$\frac{\log C(\mathbf{q})}{V} = \sum_\alpha q^\alpha \mathcal{A}_\alpha + \sum_\alpha q^\alpha \int_{\mathbf{k}} \int_0^1 dt \mathcal{A}_\alpha^{\mathbf{k}}(\mathbf{k} + \mathbf{q}t). \quad (11)$$

where the constant $\mathcal{A}_\alpha = \sum_{n \in \text{occ}} \int_{\mathbf{k}} \mathcal{A}_\alpha^n(\mathbf{k})$ is fixed by the known relation between the mean polarization and the Berry connection [60]. All higher moments are given by $\mathcal{A}_\alpha^{\mathbf{k}}(\mathbf{k} + \mathbf{q}) = \text{tr}[\hat{P}_{\mathbf{k}} (\hat{P}_{\mathbf{k}} \hat{P}_{\mathbf{k}+\mathbf{q}} \hat{P}_{\mathbf{k}})^{-1} \hat{P}_{\mathbf{k}} (\partial_\alpha \hat{P}_{\mathbf{k}+\mathbf{q}}) \hat{P}_{\mathbf{k}+\mathbf{q}}]$ involving the projector $\hat{P}_{\mathbf{k}} \equiv \hat{P}_{\text{occ}}(\mathbf{k})$ on all occupied bands for different $\mathbf{k}$. This result generalizes the single-band formula given in Ref. [23] to an arbitrary number of occupied bands.

Expanding Eq. (11) up to second and third order in $\mathbf{q}$, we obtain the cumulants

$$\langle \hat{X}_\alpha \hat{X}_\beta \rangle_c = V \int_{\mathbf{k}} \text{Re} \text{tr} [\hat{P}_{\text{occ}} (\partial_\alpha \hat{P}_{\text{occ}}) (\partial_\beta \hat{P}_{\text{occ}})], \quad (12)$$

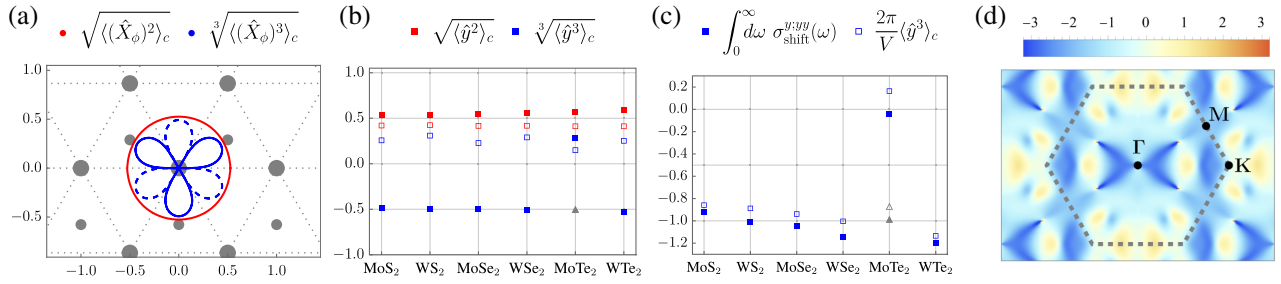


FIG. 1. (a) The roots of the variance (red) and skewness (blue) of the filled lowest band in units of the lattice constant for the transition metal dichalcogenide (TMD) MoS₂ using TNN-GGA parameters in relation to the triangular lattice of the tight-binding model (big dots). The dashed blue line indicates negative skewness. (b) The roots of the variance (red) and skewness (blue) for different TMDs comparing NN- and TNN-GGA parameters (open and filled boxes). Whereas the skewness for MoTe₂ strongly deviates using GGA parameters, a compatible value is found for LDA parameters (gray triangle). (c) The skewness of the filled band (empty boxes) yields the dominant contribution to the linear shift current sum rule (filled boxes) given in units $e^3/\hbar^2$. A clear trend for the different TMDs using TNN-GGA parameters is evident, where the TNN-LDA parameters for MoTe₂ (gray triangles) lead to better consistency. (d) The momentum-resolved contribution to the linear shift current sum rule for MoS₂ using TNN-GGA parameters, where we indicate the Brillouin zone (dashed lines) and high symmetry points.

$$\langle \hat{X}_\alpha \hat{X}_\beta \hat{X}_\gamma \rangle_c = V \int_{\mathbf{k}} \text{Im tr} \left[\hat{P}_{\text{occ}} (\partial_\alpha \hat{P}_{\text{occ}}) (\partial_\beta \partial_\gamma \hat{P}_{\text{occ}}) \right], \quad (13)$$

where V is the volume of the unit cell and $\langle \hat{X}_\alpha^2 \rangle_c = \langle (\hat{X}_\alpha - \langle \hat{X}_\alpha \rangle)^2 \rangle$ and $\langle \hat{X}_\alpha^3 \rangle_c = \langle (\hat{X}_\alpha - \langle \hat{X}_\alpha \rangle)^3 \rangle$ when focused on a single spatial direction α .

By comparing Eq. (8) with Eq. (12), we obtain that the integrated linear shift current is proportional to the skewness of the occupied states for two-band systems [46], but multistate geometry [i.e., the second term in Eq. (8)] leads to deviations in systems with more than two bands. An approximate ground-state sum rule is obtained by dropping the multiband contribution

$$\int_0^\infty d\omega \sigma_{\text{shift}}^{\alpha(\beta\gamma)}(\omega) \approx \frac{2\pi e^3}{\hbar^2} \frac{1}{V} \langle \hat{X}_\alpha \hat{X}_\beta \hat{X}_\gamma \rangle_c. \quad (14)$$

The simplified sum rule serves as an estimate for the strengths of a material's linear shift current response in terms of a straightforward ground state property, the skewness. In the next section, we quantify the accuracy of this simplification for a practical example.

Illustration for the three-band model of TMDs—We consider a single-layer of transition metal dichalcogenides (TMDs) MX₂ with M = Mo, W and X = S, Se, Te [see Fig. 1(a)]. The M atoms (big dots) form a triangular lattice used within the three-band tight-binding Hamiltonian proposed by Liu *et al.* [48]. We use their model parameters for nearest-neighbor (NN) and next-nearest-neighbor hoppings (TNN) calculated by *ab initio* density functional theory (DFT) using generalized-gradient approximation (GGA) and local-density approximation (LDA). The resulting band structure shows a lower, isolated, nondegenerate band, which we assume to be filled. The NN models capture the DFT band structure around K = (4π/3, 0), whereas the TNN models provide an overall good

agreement for all momenta [48]. We provide the details of the numerical evaluation in Supplemental Material [50]. We work in the widely used minimal tight-binding approximation, in which the off-diagonal matrix elements of the position operator are neglected; improved accuracy can be obtained either by increasing the number of bands or including off-diagonal elements [28,61].

We calculate $\langle (\hat{X}_\phi)^2 \rangle_c$ and $\langle (\hat{X}_\phi)^3 \rangle_c$ via Eqs. (12) and (13) and show their second and third root in spatial direction $\hat{X}_\phi \equiv \sin(2\pi\phi)\hat{x} + \cos(2\pi\phi)\hat{y}$ for MoS₂ centered at an M atom, which enables their comparison with the underlying lattice [see Fig. 1(a)] with lattice constant set as reference scale. The variance (red) is directionally independent, whereas the C₃ rotational symmetry becomes evident in the skewness (blue), which captures the positive tilt of the occupied states toward the nearest X atoms. We compare their amplitudes for six TMDs, sorted by increasing lattice constant, in Fig. 1(b). We see that the variance and the skewness are smaller in all NN models, which suggests a stronger M-X hybridization in the TNN models. Most importantly, the skewness obtained from the NN models has an opposite sign compared to those of the TNN models, which suggests that the longer-range hoppings over the X atoms [small dots in Fig. 1(a)] are not only required for the band dispersion but also necessary to capture essential quantum state properties due to the X atoms. As the skewness and shift current are closely related, we conclude that the NN models of TMDs are insufficient for an adequate description of the shift current and its sum rule.

We note that the result of MoTe₂ strongly deviates from the other TMDs. Since the skewness in the LDA model (gray triangle) is in line with the other TMDs, perhaps the determination of the tight-binding parameters failed for GGA, setting MoTe₂ at a potentially interesting parameter range. This discrepancy may be related to the band crossing on the M-Γ high-symmetry line seen in DFT between the

filled band and a lower band not included in the three-band description [48].

To verify the accuracy of the simplified sum rule in Eq. (14), we show $\int_0^\infty d\omega \sigma_{\text{shift}}^{yy}(\omega)$ (filled boxes) in comparison to the skewness in units $e^3/\hbar^2$ in Fig. 1(c) and find good agreement. The multistate geometry leads only to minor contributions, such that the skewness of the occupied lowest band contributes approximately 90% to the linear shift current sum rule for all TMDs. Particularly good agreement is found for MoS₂ and WTe₂. As before, only LDA model parameters for MoTe₂ follow the overall trend, whereas GGA parameters suggest a vanishing sum rule. However, we note that the multistate geometry significantly alters the momentum distribution of the sum rule integrand, as shown for MoS₂ using TNN-GGA model parameters in Fig. 1(d). The contributions at the Brillouin zone boundary (dashed lines) are mainly due to the momentum-resolved skewness. The structure around Γ is related to the multistate geometry [50]. The physical divergences on the high-symmetry line Γ -M correspond to the band crossings of the two conduction bands [50], which has no major impact on the integrated linear shift current.

Stub Rice-Mele model—To shed light on the physical origin of the multiband contributions in Eq. (8) and the validity of the sum rule (14) beyond the two-band limit, we combine the Rice-Mele model [51] with equally distant sites A and B with locally attached stubs C [52]. In the Bloch basis $(c_{k,A}^\dagger, c_{k,B}^\dagger, c_{k,C}^\dagger)$ the Bloch Hamiltonian reads

$$\hat{H}(k) = \begin{pmatrix} m & 2\cos\frac{k}{2} + 2i\delta\sin\frac{k}{2} & \Delta \\ 2\cos\frac{k}{2} - 2i\delta\sin\frac{k}{2} & -m & 0 \\ \Delta & 0 & 0 \end{pmatrix}. \quad (15)$$

Both the energy splitting m between sites A and B and the hybridization Δ between site A and the stub C are mechanisms for a finite skewness as long as the A-B chain dimerizes ($\delta \neq 0$) [50]. However, only the latter three-site mechanism leads to multiband contributions in Eq. (8), suggesting that the accuracy of the sum rule for monolayer TMDs in Fig. 1(c) arises from a dominantly two-site mechanism. The toy model indicates that multiband contributions can enhance, suppress, and even invert nonlinear optical responses. Indeed, an enhanced shift current from virtual multiband transitions has recently been suggested for alternating angle twisted multilayer graphene [62].

Conclusions and outlook—We have developed a comprehensive geometric approach to observables involving multiple band states, such as optical responses. Applying this theory to the shift current resolves the treatment of band degeneracies and establishes the precise connection between the linear shift current sum rule and the skewness of the ground state. The gauge-invariant projector formalism and techniques for its implementation, whose technical

aspects are introduced and analyzed in detail in the companion paper [49], will significantly simplify the analytic treatment of higher-order DC and optical response functions in electrical fields with charge and other current vertices, such as thermal. Responses involving the magnetic field and magnetization require a more detailed analysis due to intrinsically broken translational invariance. Another possible extension is to bands modified through light-matter coupling [63–66]. We emphasize that the multistate projector formalism does not rely on an *a priori* projection onto the low-energy sector, which simplifies a systematic identification of all leading-order contributions from real and virtual interband processes [25] and generalizes straightforwardly to some symmetry-broken phases [67]. Combining the presented approach with current attempts to avoid explicitly fixing quantum states via expansions in generators of SU(N) [44,45,49] allows for closed analytic forms of the geometric observables for more than two bands, which are needed to show pure multistate geometric effects.

The geometric analysis of low-energy tight-binding models offers a more refined characterization of the described quantum states. We revealed inconsistencies in *ab initio* models for TMDs, whose detailed analysis might lead to more refined low-energy models. Our analysis suggests that higher-order quantum geometric tensors are necessary, complementing current characterizations based on the quantum metric [68] and Berry curvature [69]. In particular, we propose to explore the validity of effective models via the amplitude and angle dependence of geometric sum rules, where the Souza-Wilkens-Martin sum rule yields information on the ground state variance [29] and the linear shift current sum rule yields information about the ground state skewness.

Studying the effect of interactions will require understanding global multistate (multimomentum) geometric objects; see, e.g., the perturbative treatment of interaction in [25]. Two promising avenues for investigation include the impact of interactions on quantization [70] and the consequences of electron-phonon coupling [71,72]. Such analyses have the potential to provide new insights into the role of vertex corrections in optical responses, which pose significant challenges for numerical methods in strongly correlated systems.

The current approach primarily aims to capture the (higher-order) local invariant objects. Note that some global geometric quantities, e.g., topological invariants, remain challenging. For example, the Zak phase of a band allows a simple representation via the Berry connection, $\phi = \int A$ and can be computed via the product of projectors along loops, but expressing it by local invariant tensors is non-trivial (Appendix G of [70]). In contrast, the multiband magnetoelectric coupling has a Chern-Simons part for which a projector expression is not known and no local, invariant representation has been found [73] without an extra dimension.

In conclusion, a comprehensive understanding of how quantum geometry determines observables will enable a more refined state tomography of quantum materials using a minimal set of observables, of which optical responses are a promising class. The formalism we presented in this Letter provides a systematic construction of the relevant geometric quantities with a given number of external indices, whose relevance has become evident from the growing number of higher-order geometric quantities [21,31,54,55,74–76]. Having identified a comprehensive set of quantum geometric tensors of different ranks, we can seek to determine the most promising observables via a careful analysis of their symmetries.

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