Computational methods for quantum geometry

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CONTENTS

I. INTRODUCTION

In these notes, we first demonstrate how one can numerically calculate the Berry curvature and quantum metric for a single isolated band and generalize this to the multiband case. To this end, we consider a gauge-invariant product of overlaps of cell-periodic Bloch functions [1]. The latter are eigenstates of the Bloch Hamiltonian:

$$\mathcal{H}_{\boldsymbol{k}} \left|u_{n\boldsymbol{k}}\right\rangle = \varepsilon_{n\boldsymbol{k}} \left|u_{n\boldsymbol{k}}\right\rangle, \tag{1}$$

with n the band index and $\boldsymbol{k}$ the crystal momentum constrained to the first Brillouin zone (BZ). In these notes, we use the normalization $\langle u_{m\boldsymbol{k}}|u_{n\boldsymbol{k}}\rangle_{\text{cell}} = \delta_{mn}$ where the overlaps are defined on the unit cell. The Bloch Hamiltonian is given by $\mathcal{H}_{\boldsymbol{k}} = e^{-i\boldsymbol{k}\cdot\boldsymbol{r}} H e^{i\boldsymbol{k}\cdot\boldsymbol{r}}$ where H is the Hamiltonian. Importantly, we work in so-called *periodic gauge* [2] where the Bloch wave functions are smoothly defined on a torus[1]:

$$\left|\psi_{n,\boldsymbol{k}+\boldsymbol{G}}\right\rangle = \left|\psi_{n\boldsymbol{k}}\right\rangle, \tag{2}$$

where $\boldsymbol{G}$ is a reciprocal lattice vector and $\left|\psi_{n\boldsymbol{k}}\right\rangle = e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} \left|u_{n\boldsymbol{k}}\right\rangle$ with $\hat{\boldsymbol{r}}$ the position operator. We thus find that

$$u_{n,\boldsymbol{k}+\boldsymbol{G}}(\boldsymbol{r}) = e^{-i\boldsymbol{G}\cdot\boldsymbol{r}} u_{n\boldsymbol{k}}(\boldsymbol{r}). \tag{3}$$

In contrast to a continuum theory, the only positional dependence in the unit cell for a lattice model comes from the sublattices. These give the centers of the basis orbitals $\boldsymbol{r}_\sigma$ where σ is a general orbital index:

$$u_{n\boldsymbol{k}}(\boldsymbol{r}) \mapsto u^\sigma_{n\boldsymbol{k}} \quad \Rightarrow \quad u^\sigma_{n,\boldsymbol{k}+\boldsymbol{G}} = e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_\sigma} u^\sigma_{n\boldsymbol{k}}. \tag{4}$$

In periodic gauge, the Bloch Hamiltonian is not periodic in momentum space. One can check that

$$\mathcal{H}_{\boldsymbol{k}+\boldsymbol{G}} = U_{\boldsymbol{G}} \mathcal{H}_{\boldsymbol{k}} U^\dagger_{\boldsymbol{G}}, \qquad U^{\sigma\sigma'}_{\boldsymbol{G}} = e^{-i\boldsymbol{G}\cdot\boldsymbol{r}_\sigma}\, \delta_{\sigma\sigma'}, \tag{5}$$

or componentwise $\mathcal{H}^{\sigma\sigma'}_{\boldsymbol{k}+\boldsymbol{G}} = e^{-i\boldsymbol{G}\cdot(\boldsymbol{r}_\sigma - \boldsymbol{r}_{\sigma'})} \mathcal{H}^{\sigma\sigma'}_{\boldsymbol{k}}$.

[1] Note that this "gauge" choice differs from the gauge choice for the overall $\boldsymbol{k}$-dependent phase, which is commonly referred to as a gauge transformation, i.e., $\left|u_{n\boldsymbol{k}}\right\rangle \mapsto e^{i\varphi_{n\boldsymbol{k}}} \left|u_{n\boldsymbol{k}}\right\rangle$ or more generally a unitary transformation if we consider a set of bands.

A. Bloch form

Instead of working in periodic gauge, we could opt to work in *Bloch form* for which the Bloch Hamiltonian is periodic in momentum space:

$$\tilde{\mathcal{H}}^{\sigma\sigma'}_{\boldsymbol{k}} = e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_\sigma - \boldsymbol{r}_{\sigma'})}\mathcal{H}^{\sigma\sigma'}_{\boldsymbol{k}}, \tag{6}$$

such that $\tilde{\mathcal{H}}_{\boldsymbol{k}+\boldsymbol{G}} = \tilde{\mathcal{H}}_{\boldsymbol{k}}$ where the tilde indicates Bloch form. In a lattice theory, this is equivalent to placing all of the orbitals in the unit cell on a single site. The cell-periodic functions in both gauges are related by

$$\tilde{u}^\sigma_{n\boldsymbol{k}} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}_\sigma} u^\sigma_{n\boldsymbol{k}}, \tag{7}$$

While this change of basis leaves the energy spectrum invariant, it affects geometrical quantities such as the Berry connection [3]. Indeed, we see that

$$\begin{aligned}
\tilde{A}^\mu_{mn} &= i\langle \tilde{u}_{m\boldsymbol{k}} | \partial^\mu \tilde{u}_{n\boldsymbol{k}} \rangle_{\text{cell}} && (8)\\
&= i\sum_\sigma \left(\tilde{u}^\sigma_{m\boldsymbol{k}}\right)^* \left(\partial^\mu \tilde{u}^\sigma_{n\boldsymbol{k}}\right) && (9)\\
&= A^\mu_{mn} - \sum_\sigma r^\mu_\sigma \left(u^\sigma_{m\boldsymbol{k}}\right)^* u^\sigma_{n\boldsymbol{k}}. && (10)
\end{aligned}$$

where $\partial^\mu = \partial/\partial k_\mu$. Similarly, the Berry curvature

$$\begin{aligned}
\tilde{F}^{\mu\nu}_n &= \partial^\mu \tilde{A}^\nu_n - \partial^\nu \tilde{A}^\mu_n && (11)\\
&= F^{\mu\nu}_n + \sum_\sigma \left(r^\mu_\sigma \partial^\nu - r^\nu_\sigma \partial^\mu\right) |u^\sigma_{n\boldsymbol{k}}|^2 && (12)\\
&= F^{\mu\nu}_n + \epsilon^{\mu\nu\alpha} \sum_\sigma \left(\boldsymbol{r}_\sigma \times \nabla_{\boldsymbol{k}}\right)_\alpha |u^\sigma_{n\boldsymbol{k}}|^2, && (13)
\end{aligned}$$

where we defined the intraband Berry connection $A^\mu_n \equiv A^\mu_{nn}$. However, note that the BZ integral of the Berry curvature is left invariant since

$$\sum_\sigma \boldsymbol{r}_\sigma \times \int d^D\boldsymbol{k}\, \nabla_{\boldsymbol{k}} |u^\sigma_{n\boldsymbol{k}}|^2 = 0, \tag{14}$$

given that $|u^\sigma_{n\boldsymbol{k}}|^2$ is always a periodic function of momentum.

Note that this basis transformation also affects other objects that involve momentum derivatives. Most notably, the velocity operator is altered. This is required since one must account for the intracell currents which would be absent if the cell has no structure. It also resolves issues that seem to arise for the anomalous linear conductivity of a metal, or the form of the semiclassical equations of motion. The latter involves the Berry curvature at a single momentum, while the former involves an integration over part of the BZ, both of which are not invariant under the basis transformation. However, the difference is exactly compensated if we use the transformed velocity operator.

II. SINGLE ISOLATED BAND

We numerically calculate the Berry curvature $\Omega_{\boldsymbol{k}} = F^{xy}_{\boldsymbol{k}}$ and Chern number for a single isolated band in $D = 2$ spatial dimension. To this end, we first consider a square plaquette of area δ^2 centered at $\boldsymbol{k}$ with corners: $\boldsymbol{k}_1 = \boldsymbol{k} + \frac{\delta}{2}(-1,-1)$, $\boldsymbol{k}_2 = \boldsymbol{k} + \frac{\delta}{2}(-1,1)$, $\boldsymbol{k}_3 = \boldsymbol{k} + \frac{\delta}{2}(1,1)$, and $\boldsymbol{k}_4 = \boldsymbol{k} + \frac{\delta}{2}(1,-1)$. When one is interested in the Berry curvature, the shape of the plaquette is not important as shown below. However, if we want to use this method to calculate the quantum metric trace, we have to use a square plaquette on a Cartesian grid. We then consider the gauge-invariant product

$$\langle u_{\boldsymbol{k}_1}|u_{\boldsymbol{k}_2}\rangle\langle u_{\boldsymbol{k}_2}|u_{\boldsymbol{k}_3}\rangle\langle u_{\boldsymbol{k}_3}|u_{\boldsymbol{k}_4}\rangle\langle u_{\boldsymbol{k}_4}|u_{\boldsymbol{k}_1}\rangle = \prod_{m=1}^{4}\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle, \tag{15}$$

where $\boldsymbol{k}_5 = \boldsymbol{k}_1$ and we dropped the band index since we consider a single band. Here, all expectation values are taken with respect to the unit cell with normalization $\langle u_{\boldsymbol{k}}|u_{\boldsymbol{k}}\rangle = 1$. Using the shorthand $\partial^\mu = \partial/\partial k_\mu$, we expand the different factors up to second order in δ as,

$$\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle = \left[\langle u_{\boldsymbol{k}}| + \delta k_{m,\mu}\partial^\mu\langle u_{\boldsymbol{k}}| + \frac{1}{2}\delta k_{m,\mu}\delta k_{m,\nu}\partial^\mu\partial^\nu\langle u_{\boldsymbol{k}}| + \mathcal{O}(\delta^3)\right] \tag{16}$$

$$\times\left[|u_{\boldsymbol{k}}\rangle + \delta k_{m+1,\mu}\partial^\mu|u_{\boldsymbol{k}}\rangle + \frac{1}{2}\delta k_{m+1,\mu}\delta k_{m+1,\nu}\partial^\mu\partial^\nu|u_{\boldsymbol{k}}\rangle + \mathcal{O}(\delta^3)\right] \tag{17}$$

$$= 1 + (\delta k_{m+1,\mu} - \delta k_{m,\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle + \delta k_{m,\mu}\delta k_{m+1,\nu}\langle\partial^\mu u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle \tag{18}$$

$$+ \frac{1}{2}\delta k_{m,\mu}\delta k_{m,\nu}\langle\partial^\mu\partial^\nu u_{\boldsymbol{k}}|u_{\boldsymbol{k}}\rangle + \frac{1}{2}\delta k_{m+1,\mu}\delta k_{m+1,\nu}\langle u_{\boldsymbol{k}}|\partial^\mu\partial^\nu u_{\boldsymbol{k}}\rangle + \mathcal{O}(\delta^3), \tag{19}$$

where we used $\langle\partial^\mu u_{\boldsymbol{k}}|u_{\boldsymbol{k}}\rangle = -\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle$. We obtain

$$\prod_{m=1}^{4}\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle = 1 + \sum_{m=1}^{4}(\delta k_{m+1,\mu} - \delta k_{m,\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle + \sum_{m=1}^{4}\delta k_{m,\mu}\delta k_{m+1,\nu}\langle\partial^\mu u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle \tag{20}$$

$$+ \frac{1}{2}\sum_{m=1}^{4}\delta k_{m,\mu}\delta k_{m,\nu}\left(\langle\partial^\mu\partial^\nu u_{\boldsymbol{k}}|u_{\boldsymbol{k}}\rangle + \langle u_{\boldsymbol{k}}|\partial^\mu\partial^\nu u_{\boldsymbol{k}}\rangle\right) \tag{21}$$

$$+ (\delta k_{2\mu} - \delta k_{1\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle(\delta k_{3\nu} - \delta k_{2\nu} + \delta k_{4\nu} - \delta k_{3\nu} + \delta k_{1\nu} - \delta k_{4\nu})\langle u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle \tag{22}$$

$$+ (\delta k_{3\mu} - \delta k_{2\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle(\delta k_{4\nu} - \delta k_{3\nu} + \delta k_{1\nu} - \delta k_{4\nu})\langle u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle \tag{23}$$

$$+ (\delta k_{4\mu} - \delta k_{3\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle(\delta k_{1\nu} - \delta k_{4\nu})\langle u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle + \mathcal{O}(\delta^4) \tag{24}$$

$$= 1 + \sum_{m=1}^{4}\delta k_{m,\mu}\delta k_{m+1,\nu}\langle\partial^\mu u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle \tag{25}$$

$$- \frac{1}{2}\sum_{m=1}^{4}\delta k_{m,\mu}\delta k_{m,\nu}\left(\langle\partial^\mu u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle + \langle\partial^\nu u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle\right) \tag{26}$$

$$+ (\delta k_{2\mu} - \delta k_{1\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle(\delta k_{1\nu} - \delta k_{2\nu})\langle u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle \tag{27}$$

$$+ (\delta k_{3\mu} - \delta k_{2\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle(\delta k_{1\nu} - \delta k_{3\nu})\langle u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle \tag{28}$$

$$+ (\delta k_{4\mu} - \delta k_{3\mu})\langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle(\delta k_{1\nu} - \delta k_{4\nu})\langle u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle + \mathcal{O}(\delta^4), \tag{29}$$

where we used

$$\langle\partial^\mu\partial^\nu u_{\boldsymbol{k}}|u_{\boldsymbol{k}}\rangle + \langle u_{\boldsymbol{k}}|\partial^\mu\partial^\nu u_{\boldsymbol{k}}\rangle = -\left(\langle\partial^\mu u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle + \langle\partial^\nu u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle\right). \tag{30}$$

For the square plaquette, we further have

$$\sum_{m=1}^{4}\delta k_{m,\mu}\delta k_{m,\nu} = \delta^2\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \qquad \sum_{m=1}^{4}\delta k_{m,\mu}\delta k_{m+1,\nu} = \delta^2\begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}, \tag{31}$$

and

$$\delta\boldsymbol{k}_2 - \delta\boldsymbol{k}_1 = \delta\boldsymbol{k}_3 - \delta\boldsymbol{k}_4 = \delta(0,1), \tag{32}$$

$$\delta\boldsymbol{k}_4 - \delta\boldsymbol{k}_1 = \delta\boldsymbol{k}_3 - \delta\boldsymbol{k}_2 = \delta(1,0), \tag{33}$$

$$\delta\boldsymbol{k}_3 - \delta\boldsymbol{k}_1 = \delta(1,1). \tag{34}$$

This yields

$$\prod_{m=1}^{4}\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle = 1 - \delta^2\left(\langle\partial_{k_x}u_{\boldsymbol{k}}|\partial_{k_y}u_{\boldsymbol{k}}\rangle - \langle\partial_{k_y}u_{\boldsymbol{k}}|\partial_{k_x}u_{\boldsymbol{k}}\rangle\right) \tag{35}$$

$$- \delta^2\left(\langle\partial_{k_x}u_{\boldsymbol{k}}|\partial_{k_x}u_{\boldsymbol{k}}\rangle + \langle\partial_{k_y}u_{\boldsymbol{k}}|\partial_{k_y}u_{\boldsymbol{k}}\rangle + \langle u_{\boldsymbol{k}}|\partial_{k_x}u_{\boldsymbol{k}}\rangle^2 + \langle u_{\boldsymbol{k}}|\partial_{k_y}u_{\boldsymbol{k}}\rangle^2\right) + \mathcal{O}(\delta^4) \tag{36}$$

$$= 1 - \delta^2(\operatorname{tr} g_{\boldsymbol{k}} - i\Omega_{\boldsymbol{k}}) + \mathcal{O}(\delta^4). \tag{37}$$

Here

$$g^{\mu\nu}_{\boldsymbol{k}} = \mathrm{Re}\left(\langle\partial^\mu u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle\right) + \langle u_{\boldsymbol{k}}|\partial^\mu u_{\boldsymbol{k}}\rangle\langle u_{\boldsymbol{k}}|\partial^\nu u_{\boldsymbol{k}}\rangle, \tag{38}$$

$$\Omega_{\boldsymbol{k}} = i\left(\langle\partial_{k_x} u_{\boldsymbol{k}}|\partial_{k_y} u_{\boldsymbol{k}}\rangle - \langle\partial_{k_y} u_{\boldsymbol{k}}|\partial_{k_x} u_{\boldsymbol{k}}\rangle\right) = -2\,\mathrm{Im}\left(\langle\partial_{k_x} u_{\boldsymbol{k}}|\partial_{k_y} u_{\boldsymbol{k}}\rangle\right), \tag{39}$$

is the (single band) Fubini-Study quantum metric with $\mathrm{tr}\, g_{\boldsymbol{k}} = g^{xx}_{\boldsymbol{k}} + g^{yy}_{\boldsymbol{k}}$ and Berry curvature, respectively. They form the real and imaginary components of the (single band) quantum geometric tensor,

$$Q^{\mu\nu}_{\boldsymbol{k}} = \langle\partial^\mu u_{\boldsymbol{k}}|\left(1 - |u_{\boldsymbol{k}}\rangle\langle u_{\boldsymbol{k}}|\right)|\partial^\nu u_{\boldsymbol{k}}\rangle = g^{\mu\nu}_{\boldsymbol{k}} - \frac{i}{2}\,\epsilon^{\mu\nu}\Omega_{\boldsymbol{k}}, \tag{40}$$

where the projector ensures invariance under gauge transformations $|u_{\boldsymbol{k}}\rangle \mapsto e^{i\varphi_{\boldsymbol{k}}}|u_{\boldsymbol{k}}\rangle$. We finally obtain

$$\mathrm{tr}\, g_{\boldsymbol{k}} = \lim_{\delta\to 0}\delta^{-2}\,\mathrm{Re}\left(1 - \prod_{m=1}^{4}\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle\right) \tag{41}$$

$$= -\lim_{\delta\to 0}\delta^{-2}\,\ln\left|\prod_{m=1}^{4}\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle\right|, \tag{42}$$

$$\Omega_{\boldsymbol{k}} = \lim_{\delta\to 0}\delta^{-2}\,\arg\prod_{m=1}^{4}\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle. \tag{43}$$

A. Alternative derivation for the Berry curvature

The Berry curvature can be calculated from the Berry phase around a small plaquette:

$$\oint_{C^\delta_{\boldsymbol{k}}} d\boldsymbol{k}'\cdot\boldsymbol{A}_{\boldsymbol{k}'} = \int_{k_x-\frac{\delta}{2}}^{k_x+\frac{\delta}{2}} dk'_x\left[A_x\left(k'_x, k_y+\frac{\delta}{2}\right) - A_x\left(k'_x, k_y-\frac{\delta}{2}\right)\right] \tag{44}$$

$$+\int_{k_y-\frac{\delta}{2}}^{k_y+\frac{\delta}{2}} dk'_y\left[A_y\left(k_x-\frac{\delta}{2}, k'_y\right) - A_y\left(k_x+\frac{\delta}{2}, k'_y\right)\right] \tag{45}$$

$$= -\delta^2\left(\frac{\partial A_y}{\partial k_x} - \frac{\partial A_x}{\partial k_y}\right) + \mathcal{O}(\delta^4), \tag{46}$$

with $\boldsymbol{A}_{\boldsymbol{k}} = i\langle u_{\boldsymbol{k}}|\nabla_{\boldsymbol{k}} u_{\boldsymbol{k}}\rangle$ the Berry connection. Here $C^\delta_{\boldsymbol{k}}$ is a square contour with area δ^2 centered around $\boldsymbol{k}$ that is traversed in clockwise order. More specifically, $C^\delta_{\boldsymbol{k}} = \{\boldsymbol{k}_1 \to \boldsymbol{k}_2 \to \boldsymbol{k}_3 \to \boldsymbol{k}_4 \to \boldsymbol{k}_1\}$ with $\boldsymbol{k}_1 = \boldsymbol{k} + \frac{\delta}{2}(-1,-1)$, $\boldsymbol{k}_2 = \boldsymbol{k} + \frac{\delta}{2}(-1,1)$, $\boldsymbol{k}_3 = \boldsymbol{k} + \frac{\delta}{2}(1,1)$, and $\boldsymbol{k}_4 = \boldsymbol{k} + \frac{\delta}{2}(1,-1)$. Hence

$$\Omega_{\boldsymbol{k}} = \lim_{\delta\to 0}\delta^{-2}\arg\exp\left(-i\oint_{C^\delta_{\boldsymbol{k}}} d\boldsymbol{k}'\cdot\boldsymbol{A}_{\boldsymbol{k}'}\right). \tag{47}$$

The Berry phase is then calculated numerically as follows,

$$\arg e^{-i\sum_{m=1}^{4}(\boldsymbol{k}_{m+1}-\boldsymbol{k}_m)\cdot\boldsymbol{A}_{\boldsymbol{k}_m}} = \arg\prod_{m=1}^{4}\left[1 - i\left(\boldsymbol{k}_{m+1}-\boldsymbol{k}_m\right)\cdot\boldsymbol{A}_{\boldsymbol{k}_m}\right] = \arg\prod_{m=1}^{4}\langle u_{\boldsymbol{k}_m}|u_{\boldsymbol{k}_{m+1}}\rangle, \tag{48}$$

with $\boldsymbol{k}_5 = \boldsymbol{k}_1$ and which holds up to order δ^2. One can show explicitly that the leading-order term on the right-hand side gives $\delta^2\Omega_{\boldsymbol{k}}$ (see above derivation). We thus find again that

$$\Omega_{\boldsymbol{k}} = \lim_{\delta\to 0}\delta^{-2}\arg\left(\langle u_{\boldsymbol{k}_1}|u_{\boldsymbol{k}_2}\rangle\langle u_{\boldsymbol{k}_2}|u_{\boldsymbol{k}_3}\rangle\langle u_{\boldsymbol{k}_3}|u_{\boldsymbol{k}_4}\rangle\langle u_{\boldsymbol{k}_4}|u_{\boldsymbol{k}_1}\rangle\right). \tag{49}$$

B. Transformation law

How does the quantum metric and Berry curvature transform under a change of coordinates? To this end, we consider a Bravais grid

$$\boldsymbol{k} = k_1\boldsymbol{G}_1 + k_2\boldsymbol{G}_2 = \underline{G}\begin{pmatrix}k_1\\k_2\end{pmatrix}, \tag{50}$$

with $\underline{G} = \begin{pmatrix} \boldsymbol{G}_1 & \boldsymbol{G}_2 \end{pmatrix}$. If we denote the Bravais indices with $i, j = 1, 2$ and Cartesian coordinates with $\mu, \nu = x, y$, we find that

$$g^{\mu\nu}_{\boldsymbol{k}} = \underline{G}^{\mu}_{i} \underline{G}^{\nu}_{j} g^{ij}_{\boldsymbol{k}}, \tag{51}$$

$$F^{xy}_{\boldsymbol{k}} = \det\left(\underline{G}\right) F^{12}_{\boldsymbol{k}} = V_{\mathrm{BZ}} F^{12}_{\boldsymbol{k}}, \tag{52}$$

with $V_{\mathrm{BZ}} = (2\pi)^2 / V_{\mathrm{cell}}$ the area of the first Brillouin zone. Because in general $\underline{G}$ is not an orthogonal matrix, the trace of the quantum metric is not invariant under this transformation. Hence we can calculate the Berry curvature from the gauge-invariant product up to a multiplicative constant with a Bravais grid or even for a different contour, such as a triangle instead of a square. However, the trace of the quantum metric is not invariant and we need to take a square Cartesian grid.

C. Example: Haldane model

The Bloch Hamiltonian of a two-band system can be written as

$$\mathcal{H} = \boldsymbol{d}(\boldsymbol{k}) \cdot \boldsymbol{\sigma} = d(\boldsymbol{k}) \left[P_{+}(\boldsymbol{k}) - P_{-}(\boldsymbol{k}) \right], \tag{53}$$

with $d = |\boldsymbol{d}|$ and

$$P_{\pm} = \frac{1}{2} \left(\mathbb{1}_2 \pm \boldsymbol{n} \cdot \boldsymbol{\sigma} \right), \tag{54}$$

the projectors on the bands where $\boldsymbol{n} = \boldsymbol{d}/d$ is unit vector. You can check that $P_{\pm}^2 = P_{\pm}$ since $(\boldsymbol{n} \cdot \boldsymbol{\sigma})^2 = \mathbb{1}_2$. Setting $d(\boldsymbol{k}) = 1$ corresponds to flattening of the bands, which preserves the quantum-geometric and topological properties which are given solely in terms of $\boldsymbol{n}$.

The quantum metric is obtained from [see Eq. (127) below]

$$\mathrm{Tr}\left[\left(\delta P_{\boldsymbol{k}} \right)^2 \right] = 2 g^{\mu\nu}_{\boldsymbol{k}} dk_{\mu} dk_{\nu}, \tag{55}$$

where $\delta P_{\boldsymbol{k}} = \left(P_{\boldsymbol{k}+d\boldsymbol{k}} - P_{\boldsymbol{k}-d\boldsymbol{k}} \right)/2$. In this case, we find

$$\mathrm{Tr}\left[\left(\delta P_{\pm} \right)^2 \right] = \frac{1}{4} \mathrm{Tr}\left[\left(\partial^{\mu} \boldsymbol{n} \cdot \boldsymbol{\sigma} \right) \left(\partial^{\nu} \boldsymbol{n} \cdot \boldsymbol{\sigma} \right) \right] dk_{\mu} dk_{\nu} \tag{56}$$

$$= \frac{1}{2} \left(\partial^{\mu} \boldsymbol{n} \right) \cdot \left(\partial^{\nu} \boldsymbol{n} \right) dk_{\mu} dk_{\nu}, \tag{57}$$

such that

$$g^{\mu\nu}_{\boldsymbol{k}} = \frac{1}{4} \left(\partial^{\mu} \boldsymbol{n} \right) \cdot \left(\cdot \partial^{\nu} \boldsymbol{n} \right). \tag{58}$$

One can show from a tedious but straightforward direct calculation that the Berry curvature is given by

$$\Omega_{\boldsymbol{k}} = \frac{1}{2} \boldsymbol{n} \cdot \left(\partial^{x} \boldsymbol{n} \times \partial^{y} \boldsymbol{n} \right), \tag{59}$$

which corresponds to the Jacobian determinant of the map $\boldsymbol{n} : T^2 \mapsto S^2$ from the BZ torus to the Bloch sphere. Its integral is then given by the wrapping number which gives the Chern number. For the Haldane model, we have

$$d_1 = \mathrm{Re}\, f(\boldsymbol{k}), \tag{60}$$

$$d_2 = \mathrm{Im}\, f(\boldsymbol{k}), \tag{61}$$

$$d_3 = m_0 + m_1 g(\boldsymbol{k}), \tag{62}$$

with

$$f(\boldsymbol{k}) = \sum_{n=1}^{3} e^{i \boldsymbol{k} \cdot \boldsymbol{\delta}_n}, \tag{63}$$

$$g(\boldsymbol{k}) = \frac{2}{\sqrt{3}} \left\{ \sin\left(\boldsymbol{k} \cdot \boldsymbol{a}_1 \right) - \sin\left(\boldsymbol{k} \cdot \boldsymbol{a}_2 \right) - \sin\left[\left(\boldsymbol{k} \cdot \left(\boldsymbol{a}_1 - \boldsymbol{a}_2 \right) \right) \right] \right\}, \tag{64}$$

with $\boldsymbol{\delta}_n = R(2\pi/3)^{n-1} \left(0, a/\sqrt{3} \right)$ and lattice constant a.

D. In terms of velocity matrix elements

We can also express the quantum geometric tensor in terms of the band off-diagonal velocity matrix elements by adding a complete set. Starting from the definition, we find

$$Q^{\mu\nu}_{n\boldsymbol{k}} = \langle\partial^\mu u_{n\boldsymbol{k}}|\partial^\nu u_{n\boldsymbol{k}}\rangle + \langle u_{n\boldsymbol{k}}|\partial^\nu u_{n\boldsymbol{k}}\rangle\langle u_{n\boldsymbol{k}}|\partial^\nu u_{n\boldsymbol{k}}\rangle \tag{65}$$

$$= \sum_m \langle\partial^\mu u_{n\boldsymbol{k}}|u_{m\boldsymbol{k}}\rangle\langle u_{m\boldsymbol{k}}|\partial^\nu u_{n\boldsymbol{k}}\rangle + \langle u_{n\boldsymbol{k}}|\partial^\nu u_{n\boldsymbol{k}}\rangle\langle u_{n\boldsymbol{k}}|\partial^\nu u_{n\boldsymbol{k}}\rangle \tag{66}$$

$$= -\sum_{m\neq n} \langle u_{n\boldsymbol{k}}|\partial^\mu u_{m\boldsymbol{k}}\rangle\langle u_{m\boldsymbol{k}}|\partial^\nu u_{n\boldsymbol{k}}\rangle \tag{67}$$

$$= \sum_{m\neq n} \frac{\langle u_{n\boldsymbol{k}}|\left(\partial^\mu\mathcal{H}\right)|u_{m\boldsymbol{k}}\rangle\langle u_{m\boldsymbol{k}}|\left(\partial^\nu\mathcal{H}\right)|u_{n\boldsymbol{k}}\rangle}{\left(\varepsilon_{m\boldsymbol{k}}-\varepsilon_{n\boldsymbol{k}}\right)^2} \tag{68}$$

where we made use of $\mathcal{H}\,|u_{n\boldsymbol{k}}\rangle = \varepsilon_{n\boldsymbol{k}}\,|u_{n\boldsymbol{k}}\rangle$ and hence

$$\left(\partial^\mu\mathcal{H} - \partial^\mu\varepsilon_{n\boldsymbol{k}}\right)|u_{n\boldsymbol{k}}\rangle = \left(\varepsilon_{n\boldsymbol{k}}-\mathcal{H}\right)|\partial^\mu u_{n\boldsymbol{k}}\rangle\,, \tag{69}$$

such that

$$\langle u_{m\boldsymbol{k}}|\left(\partial^\mu\mathcal{H}\right)|u_{n\boldsymbol{k}}\rangle = \delta_{mn}\partial^\mu\varepsilon_{n\boldsymbol{k}} + \left(\varepsilon_{n\boldsymbol{k}}-\varepsilon_{m\boldsymbol{k}}\right)\langle u_{m\boldsymbol{k}}|\,\partial^\mu u_{n\boldsymbol{k}}\rangle. \tag{70}$$

III. MULTIBAND CASE

A. Berry curvature

We consider an isolated band manifold that contains N bands with cell-periodic Bloch functions

$$U_{\boldsymbol{k}} = \left(|u_{1\boldsymbol{k}}\rangle\ \ |u_{2\boldsymbol{k}}\rangle\ \ \cdots\ \ |u_{N\boldsymbol{k}}\rangle\right), \tag{71}$$

which is a $M\times N$ matrix where M is the total number of bands, and such that $U^\dagger U = \mathbb{1}_N$. We now define the connection 1-form

$$\mathcal{A} = U^\dagger dU = U^\dagger\,\frac{\partial U}{\partial k_\mu}\,dk_\mu, \tag{72}$$

such that the components $\mathcal{A}^\mu = U^\dagger\partial^\mu U$ are given by $N\times N$ anti-Hermitian matrices with components

$$\mathcal{A}^\mu_{mn} = \langle u_{m\boldsymbol{k}}|\partial^\mu u_{n\boldsymbol{k}}\rangle. \tag{73}$$

Under a unitary transformation $U\mapsto UX$ where X is a $N\times N$ unitary matrix that acts in the subspace spanned by the N bands. We find that the connection is not covariant under this unitary transformation:

$$\mathcal{A}\mapsto X^\dagger\mathcal{A}X + X^\dagger\,\frac{\partial X}{\partial k_\mu}\,dk_\mu = X^\dagger\mathcal{A}X + X^\dagger dX. \tag{74}$$

However, we can define the Wilczek-Zee curvature which is a covariant 2-form

$$\mathcal{F} = d\mathcal{A} + \mathcal{A}\wedge\mathcal{A} \tag{75}$$

$$= \left(\frac{\partial\mathcal{A}^\nu}{\partial k_\mu} + \frac{1}{2}\left[\mathcal{A}^\mu,\mathcal{A}^\nu\right]\right)dk_\mu\wedge dk_\nu \tag{76}$$

$$= \frac{1}{2}\,\mathcal{F}^{\mu\nu}\,dk_\mu\wedge dk_\nu, \tag{77}$$

with component matrices

$$\mathcal{F}^{\mu\nu} = -\mathcal{F}^{\nu\mu} = \frac{\partial\mathcal{A}^\nu}{\partial k_\mu} - \frac{\partial\mathcal{A}^\mu}{\partial k_\nu} + \left[\mathcal{A}^\mu,\mathcal{A}^\nu\right]. \tag{78}$$

To show that it transforms covariantly, we let $U \mapsto UX$ and consider the antisymmetric part of

$$\partial^\mu \left(X^\dagger \mathcal{A}^\nu X + X^\dagger \partial^\nu X\right) + \frac{1}{2} X^\dagger [\mathcal{A}^\mu, \mathcal{A}^\nu] X + \frac{1}{2} \left([X^\dagger \partial^\mu X, X^\dagger \mathcal{A}^\nu X] + [X^\dagger \mathcal{A}^\mu X, X^\dagger \partial^\nu X] + [X^\dagger \partial^\mu X, X^\dagger \partial^\nu X]\right), \quad (79)$$

with

$$[X^\dagger \partial^\mu X, X^\dagger \partial^\nu X] = X^\dagger \left(\partial^\mu X\right) X^\dagger \left(\partial^\nu X\right) - X^\dagger \left(\partial^\nu X\right) X^\dagger \left(\partial^\mu X\right) \quad (80)$$

$$= -\left(\left(\partial^\mu X\right)^\dagger \left(\partial^\nu X\right) - \left(\partial^\nu X\right)^\dagger \left(\partial^\mu X\right)\right), \quad (81)$$

where we used $X^\dagger \left(\partial^\mu X\right) = -\left(\partial^\mu X\right)^\dagger X$ since X is unitary. We see that these terms cancel with the second term of Eq. (79), namely $\partial^\mu \left(X^\dagger \partial^\nu X\right)$ since we consider only the antisymmetric part. Likewise, we find

$$[X^\dagger \partial^\mu X, X^\dagger \mathcal{A}^\nu X] = X^\dagger \left(\partial^\mu X\right) X^\dagger \mathcal{A}^\nu X - X^\dagger \mathcal{A}^\nu \left(\partial^\mu X\right) \quad (82)$$

$$= -\left(\partial^\mu X\right)^\dagger \mathcal{A}^\nu X - X^\dagger \mathcal{A}^\nu \left(\partial^\mu X\right), \quad (83)$$

$$[X^\dagger \mathcal{A}^\mu X, X^\dagger \partial^\nu X] = X^\dagger \mathcal{A}^\mu \left(\partial^\nu X\right) - X^\dagger \left(\partial^\nu X\right) X^\dagger \mathcal{A}^\mu X \quad (84)$$

$$= X^\dagger \mathcal{A}^\mu \left(\partial^\nu X\right) + \left(\partial^\nu X\right)^\dagger \mathcal{A}^\mu X. \quad (85)$$

We thus conclude that $\mathcal{F}$ is gauge covariant:

$$\mathcal{F} \mapsto X^\dagger \mathcal{F} X, \quad (86)$$

such that the Berry curvature $F = i \operatorname{Tr} \mathcal{F}$ is gauge invariant, where the trace runs over the N isolated bands under consideration. Note that

$$F = \frac{i}{2} \operatorname{Tr}\left(\mathcal{F}^{\mu\nu}\right) dk_\mu \wedge dk_\nu, \quad (87)$$

or explicitly,

$$F^{\mu\nu} = i \operatorname{Tr}\left(\mathcal{F}^{\mu\nu}\right) = i \sum_{n=1}^{N} \left(\langle \partial^\mu u_{n\boldsymbol{k}} | \partial^\nu u_{n\boldsymbol{k}} \rangle - \langle \partial^\nu u_{n\boldsymbol{k}} | \partial^\mu u_{n\boldsymbol{k}} \rangle\right), \quad (88)$$

since $\operatorname{Tr}\left(\mathcal{A} \times \mathcal{A}\right) = 0$. Since the trace is linear, it commutes with the exterior derivative. We can thus also write

$$F = i \operatorname{Tr}\left(d\mathcal{A}\right) = dA, \quad (89)$$

with $A = i \operatorname{Tr}\left(\mathcal{A}\right)$ the Berry connection.

B. Wilson loop

The Wilson loop is a generalization of the Berry phase for N isolated bands. Since the bands are isolated, there is a finite energy gap to all other bands, while the energy gap between the constituent bands is allowed to vanish. To define the Wilson loop, we first consider a closed path $\mathcal{C}$ in the BZ. The Wilson loop along $\mathcal{C}$ is then defined as

$$\mathcal{W}(\mathcal{C}) = \mathcal{P} \exp\left[\oint_{\mathcal{C}} dk_\mu \, \mathcal{A}^\mu\right], \quad (90)$$

which is a $N \times N$ unitary matrix and where $\mathcal{P}$ denotes path ordering. We further defined the matrix of Berry connections $\mathcal{A}^\mu = U^\dagger \partial^\mu U$ of the isolated manifold of bands (note that we omit the factor of i here). If we want to calculate the Wilson loop numerically, we need to discretize the loop $\mathcal{C}$. For a loop at $\boldsymbol{k}_1$, consider the discretization $\{\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_n\}$ where $\boldsymbol{k}_n = \boldsymbol{k}_1$. The discretized Wilson loop along $\mathcal{C}$ is then defined as

$$\mathcal{W}_n(\mathcal{C}) = U_1^\dagger U_2 U_2^\dagger U_3 \cdots U_{n-1}^\dagger U_n, \quad (91)$$

where $U_{\boldsymbol{k}}$ is the matrix of cell-periodic Bloch eigenstates of the N isolated bands at $\boldsymbol{k}$. The discretized Wilson loop is not unitary in general because $U^\dagger U = \mathbb{1}_N$ but $P = UU^\dagger$. In the limit $n \to \infty$, Eq. (91) becomes exact and $\mathcal{W}(\mathcal{C}) = \lim_{n\to\infty} \mathcal{W}_n(\mathcal{C})$. The total Berry phase around the loop $\mathcal{C}$ is defined as the argument of the sum of the eigenvalues of $\mathcal{W}(\mathcal{C})$

$$\phi(\mathcal{C}) \equiv i \, \ln\det\left[\mathcal{W}(\mathcal{C})\right] = i \oint_{\mathcal{C}} dk^\mu \operatorname{Tr}\left(\mathcal{A}^\mu\right) = \oint_{\mathcal{C}} dk^\mu \, A^\mu, \quad (92)$$

where $\operatorname{Tr}\left(\mathcal{A}^\mu\right)$ is purely imaginary. For the discretized Wilson loop, we define

$$\phi_n(\mathcal{C}) = -\arg\det\left[\mathcal{W}_n(\mathcal{C})\right] = -N \arg\operatorname{Tr}\left[\mathcal{W}_n(\mathcal{C})\right]. \quad (93)$$

C. Quantum geometric tensor

In general, the quantum geometric tensor for N isolated bands is defined as (see e.g. [4] for a recent work)

$$\mathcal{Q}^{\mu\nu}_{mn}(\boldsymbol{k}) = \langle \partial^\mu u_{m\boldsymbol{k}} | \, 1 - P_{\boldsymbol{k}} \, | \partial^\nu u_{n\boldsymbol{k}} \rangle \,, \tag{94}$$

with $P_{\boldsymbol{k}} = \sum_{n=1}^{N} |u_{n\boldsymbol{k}}\rangle \langle u_{n\boldsymbol{k}}|$ the projector on the isolated band manifold. The projector ensures that $\mathcal{Q}^{\mu\nu}$ is gauge covariant under a unitary transformation of the bands. In matrix notation and dropping the momentum index, we have $P = UU^\dagger$ and

$$\mathcal{Q}^{\mu\nu} = (\partial^\mu U)^\dagger \left(\mathbb{1}_M - UU^\dagger\right) (\partial^\nu U) \,, \tag{95}$$

with M the total number of bands. Under a unitary transformation $U \mapsto UX$, and we find

$$\begin{aligned}
\mathcal{Q}^{\mu\nu} \mapsto \; & X^\dagger \mathcal{Q}^{\mu\nu} X && (96)\\
& + (U\partial^\mu X)^\dagger \left(\mathbb{1}_M - UU^\dagger\right) (\partial^\nu U) \, X && (97)\\
& + X^\dagger \, (\partial^\mu U)^\dagger \left(\mathbb{1}_M - UU^\dagger\right) U \partial^\nu X && (98)\\
& + (U\partial^\mu X)^\dagger \left(\mathbb{1}_M - UU^\dagger\right) U \partial^\nu X = X^\dagger \mathcal{Q}^{\mu\nu} X, && (99)
\end{aligned}$$

where we used that $U^\dagger U = \mathbb{1}_N$. We can therefore define the gauge-invariant trace over bands,

$$Q^{\mu\nu} = \mathrm{Tr}\,(\mathcal{Q}^{\mu\nu}) = G^{\mu\nu} - \frac{i}{2} F^{\mu\nu}, \tag{100}$$

which we have written in terms of its real and imaginary part. We further find that since $(\mathcal{Q}^{\mu\nu})^\dagger = \mathcal{Q}^{\nu\mu}$, the trace satisfies $(Q^{\mu\nu})^* = Q^{\nu\mu}$. Hence the real part $G^{\mu\nu} = G^{\nu\mu}$, i.e., the quantum metric, is symmetric in the momentum indices, while for the imaginary part we find $F^{\mu\nu} = -F^{\nu\mu}$. The imaginary part is given by the Berry curvature:

$$\begin{aligned}
F^{\mu\nu} = i \, (Q^{\mu\nu} - Q^{\nu\mu}) &= i \sum_{n=1}^{N} \left[\langle \partial^\mu u_n | \, 1 - P \, | \partial^\nu u_n \rangle - (\mu \leftrightarrow \nu) \right] && (101)\\
&= i \sum_{n=1}^{N} \left[\langle \partial^\mu u_n | \partial^\nu u_n \rangle - (\mu \leftrightarrow \nu) \right], && (102)
\end{aligned}$$

since making use of the normalization $\langle u_m | u_n \rangle = \delta_{mn}$ we have that

$$\langle \partial^\mu u_n | u_m \rangle \langle u_m | \partial^\nu u_n \rangle = \langle \partial^\nu u_m | u_n \rangle \langle u_n | \partial^\mu u_m \rangle, \tag{103}$$

which is symmetric in its momentum indices when summed over m and n. Hence the multiband Berry curvature is given by the sum of the Berry curvature of the individual bands. The quantum metric is then given by

$$\begin{aligned}
G^{\mu\nu} = \frac{1}{2} \, (Q^{\mu\nu} + Q^{\nu\mu}) &= \frac{1}{2} \sum_{n=1}^{N} \left[\langle \partial^\mu u_n | \, 1 - P \, | \partial^\nu u_n \rangle + (\mu \leftrightarrow \nu) \right] && (104)\\
&= \sum_{n=1}^{N} \left[\mathrm{Re}\left(\langle \partial^\mu u_n | \partial^\nu u_n \rangle \right) - \sum_{m=1}^{N} \langle \partial^\mu u_n | u_m \rangle \langle u_m | \partial^\nu u_n \rangle \right] && (105)\\
&= \sum_{n=1}^{N} \left[\mathrm{Re}\left(\langle \partial^\mu u_n | \partial^\nu u_n \rangle \right) - \sum_{m=1}^{N} \mathcal{A}^\mu_{nm} \mathcal{A}^\nu_{mn} \right], && (106)
\end{aligned}$$

which is *not* equal to the sum of the quantum metric of the individual bands.

We now want to show that we can numerically calculate $\mathrm{tr}\,(G) = G^{xx} + G^{yy}$ and $\Omega = F^{xy}$ for the multiband case in $D = 2$ spatial dimensions from the gauge-covariant matrix product:

$$U_1^\dagger U_2 U_2^\dagger U_3 U_3^\dagger U_4 U_4^\dagger U_1 = \prod_{m=1}^{4} U_m^\dagger U_{m+1}, \tag{107}$$

with $U_5 = U_1$. Similarly as before, using that $U^\dagger U = \mathbb{1}_N$, we find

$$U_m^\dagger U_{m+1} = \mathbb{1}_N + (\delta k_{m+1,\mu} - \delta k_{m,\mu})\, U^\dagger \partial^\mu U + \delta k_{m,\mu}\delta k_{m,\nu}\, (\partial^\mu U)^\dagger\, \partial^\nu U + \frac{1}{2}\delta k_{m,\mu}\delta k_{m,\nu}\, (\partial^\mu\partial^\nu U)^\dagger\, U \tag{108}$$

$$+ \frac{1}{2}\delta k_{m+1,\mu}\delta k_{m+1,\nu} U^\dagger \partial^\mu\partial^\nu U + \mathcal{O}(\delta^3), \tag{109}$$

where U is evaluated at the center of the plaquette. However, some of the following steps might not hold because the different factors in the gauge-invariant product no longer commute. We can resolve this by taking the trace over band indices instead. Under the trace, we can treat the product of two matrices [the analog of terms like those in Eq. (27)] as if they were complex numbers. Here, we also make use of

$$(\partial^\mu\partial^\nu U)^\dagger\, U + U^\dagger\, (\partial^\mu\partial^\nu U) = -\left[(\partial^\mu U)^\dagger\, (\partial^\nu U) + (\partial^\nu U)^\dagger\, (\partial^\mu U)\right], \tag{110}$$

which follows from differentiating $U^\dagger U = \mathbb{1}_N$ twice. We thus obtain

$$\mathrm{Tr}\left(\prod_{m=1}^{4} U_m^\dagger U_{m+1}\right) = N - \delta^2\, (\mathrm{tr}\, G - i\Omega) + \mathcal{O}(\delta^4), \tag{111}$$

where Tr runs over band indices and tr runs over spatial indices. This yields

$$\mathrm{tr}\, G = \lim_{\delta\to 0} \delta^{-2}\, \mathrm{Re}\left[N - \mathrm{Tr}\left(\prod_{m=1}^{4} U_m^\dagger U_{m+1}\right)\right], \tag{112}$$

$$\Omega = N \lim_{\delta\to 0} \delta^{-2}\, \arg \mathrm{Tr}\left(\prod_{m=1}^{4} U_m^\dagger U_{m+1}\right) = \lim_{\delta\to 0} \delta^{-2}\, \arg\det\left(\prod_{m=1}^{4} U_m^\dagger U_{m+1}\right). \tag{113}$$

Here we used that

$$\det\left(\mathbb{1}_N + \delta^2 M\right) = 1 + \delta^2 \mathrm{Tr}(M) + \mathcal{O}(\delta^4), \tag{114}$$

such that

$$\det\left(\prod_{m=1}^{4} U_m^\dagger U_{m+1}\right) = 1 - \delta^2\, (\mathrm{tr}\, G - i\Omega) + \mathcal{O}(\delta^4). \tag{115}$$

D. In terms of velocity matrix elements

Similarly as before, and denoting the manifold of bands as $\mathcal{M}$, we find

$$Q^{\mu\nu} = \sum_{n\in\mathcal{M}} \left[\langle\partial^\mu u_n|\partial^\nu u_n\rangle - \sum_{m\in\mathcal{M}} \langle\partial^\mu u_n|u_m\rangle\langle u_m|\partial^\nu u_n\rangle\right] \tag{116}$$

$$= \sum_{n\in\mathcal{M}} \left[\sum_{l} \langle\partial^\mu u_n|u_l\rangle\langle u_l|\partial^\nu u_n\rangle - \sum_{m\in\mathcal{M}} \langle\partial^\mu u_n|u_m\rangle\langle u_m|\partial^\nu u_n\rangle\right] \tag{117}$$

$$= \sum_{n\in\mathcal{M}} \sum_{m\notin\mathcal{M}} \langle\partial^\mu u_n|u_m\rangle\langle u_m|\partial^\nu u_n\rangle \tag{118}$$

$$= \sum_{n\in\mathcal{M}} \sum_{m\notin\mathcal{M}} \frac{\langle u_n|\, (\partial^\mu\mathcal{H})\, |u_m\rangle\langle u_m|\, (\partial^\nu\mathcal{H})\, |u_n\rangle}{(\varepsilon_m - \varepsilon_n)^2}. \tag{119}$$

Trace condition

From the right-hand side of Eq. (104), one can see that $\mathrm{tr}\, G$ is always positive, since $1 - P = \sum_{m\notin N} |u_m\rangle\, \langle u_m|$ and the diagonal entries thus only involve squared norms, together with Eq. (101) it can be shown that

$$\mathrm{tr}\, G \geq |\Omega|, \tag{120}$$

which is called the trace inequality. This result may be obtained by writing the derivatives in terms of the holomorphic derivatives $\partial = \frac{1}{2}\left(\partial_{k_x} - i\partial_{k_y}\right)$ and $\bar{\partial} = \frac{1}{2}\left(\partial_{k_x} + i\partial_{k_y}\right)$ [**?**]. When the bound is saturated at each $\boldsymbol{k}$ point, one says that the trace condition is satisfied, which is a necessary condition for perfect or ideal quantum geometry. A band that has perfect quantum geometry is equivalent to the lowest Landau level. Moreover, a manifold of bands that satisfies the trace condition as given in Eq. (120) is also called vortexable and features perfect magnetic circular dichroism. It can therefore be interesting to also plot the difference $\mathrm{tr}\,(G) - |\Omega|$ both as an extra cross check (it should be positive) and as a measure of ideal quantum geometry.

E. Alternative calculation of the multiband quantum metric

We start from the projector

$$P_{\boldsymbol{k}} = U_{\boldsymbol{k}} U_{\boldsymbol{k}}^{\dagger}, \tag{121}$$

which is a gauge-invariant $M \times M$ matrix with M the total number of bands. We then consider small changes in $P_{\boldsymbol{k}}$,

$$\delta P_{\boldsymbol{k}} = \frac{P_{\boldsymbol{k}+d\boldsymbol{k}} - P_{\boldsymbol{k}-d\boldsymbol{k}}}{2} \simeq \left[\left(\partial^{\mu} U_{\boldsymbol{k}}\right) U_{\boldsymbol{k}}^{\dagger} + U_{\boldsymbol{k}} \left(\partial^{\mu} U_{\boldsymbol{k}}\right)^{\dagger}\right] dk_{\mu}, \tag{122}$$

valid up to second order. We then find (dropping the momentum index)

$$\begin{aligned}
\mathrm{Tr}\left[(\delta P)^2\right] &\simeq \mathrm{Tr}\left\{\left[\left(\partial^{\mu} U\right) U^{\dagger} + U\left(\partial^{\mu} U\right)^{\dagger}\right]\left[\left(\partial^{\nu} U\right) U^{\dagger} + U\left(\partial^{\nu} U\right)^{\dagger}\right]\right\} dk_{\mu} dk_{\nu} && (123)\\
&= \mathrm{Tr}\left\{\left(\partial^{\mu} U\right)^{\dagger}\left(\partial^{\nu} U\right) + \left(\partial^{\nu} U\right)^{\dagger}\left(\partial^{\mu} U\right) + U^{\dagger}\left(\partial^{\mu} U\right) U^{\dagger}\left(\partial^{\nu} U\right) + \left(\partial^{\nu} U\right)^{\dagger} U \left(\partial^{\mu} U\right)^{\dagger} U\right\} dk_{\mu} dk_{\nu} && (124)\\
&= \mathrm{Tr}\left\{\left(\partial^{\mu} U\right)^{\dagger}\left(\partial^{\nu} U\right) + \left(\partial^{\nu} U\right)^{\dagger}\left(\partial^{\mu} U\right) - \left(\partial^{\mu} U\right)^{\dagger} U U^{\dagger}\left(\partial^{\nu} U\right) - \left(\partial^{\nu} U\right)^{\dagger} U U^{\dagger}\left(\partial^{\mu} U\right)\right\} dk_{\mu} dk_{\nu} && (125)\\
&= \mathrm{Tr}\left\{\left(\partial^{\mu} U\right)^{\dagger}\left(\mathbb{1}_M - U U^{\dagger}\right)\left(\partial^{\nu} U\right) + (\mu \leftrightarrow \nu)\right\} dk_{\mu} dk_{\nu} && (126)\\
&= 2 G^{\mu\nu} dk_{\mu} dk_{\nu}, && (127)
\end{aligned}$$

where we used the properties of the trace and that $U^{\dagger}U = \mathbb{1}_N$ such that $(\partial^{\mu} U)^{\dagger} U = -U^{\dagger}(\partial^{\mu} U)$. We can now take $d\boldsymbol{k} = (\delta, 0)$, $(0, \delta)$, and (δ, δ) together with the fact that $G^{\mu\nu} = G^{\nu\mu}$ to find all components of $G^{\mu\nu}$.

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