Quantum Geometric Tensor is defined by

$$M^{\mathcal{B}}_{\mu\nu}(\mathbf{k}) = 2\sum_{i\in\mathcal{B}} \langle \frac{\partial}{\partial k_\mu}\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\frac{\partial}{\partial k_\nu}\psi_{\mathbf{k}i}\rangle \tag{1}$$

$$g_{\mu\nu}(\mathbf{k}) = \frac{1}{2}(M_{\mu\nu}(\mathbf{k})+M_{\nu\mu}(\mathbf{k})) \tag{2}$$

$$\tag{3}$$

The Berry curvature is

$$\Omega_{\mu\nu} = i(M_{\mu\nu}-M_{\nu\mu}) \tag{4}$$

How is quantum metric related to distance between Bloch states? We have

$$1-|\langle\psi_{\mathbf{k}n}|\psi_{\mathbf{k}+d\mathbf{k},n}\rangle|^2 = \frac{1}{2}\sum_{\mu\nu} M^n_{\mu\nu}(\mathbf{k})dk_\mu dk_\nu \tag{5}$$

To derive this, you need to take into account both the first and the second derivative of the wave function, i.e.,

$$\psi_{\mathbf{k}+d\mathbf{k},n} \approx \psi_{\mathbf{k},n} + \sum_\mu \frac{\partial}{\partial k_\mu}\psi_{\mathbf{k},n}dk_\mu + \frac{1}{2}\sum_{\mu\nu}\frac{\partial^2}{\partial k_\mu \partial k_\nu}\psi_{\mathbf{k},n}dk_\mu dk\nu \tag{6}$$

and then the straightforward expansion leads to the above formula.

The definition is gauge invariant, in the sense that redefining single particle wave functions by an arbitrary phase

$$\widetilde{\psi}_{\mathbf{k}i}(\mathbf{r}) = e^{i\beta_i(\mathbf{k})}\psi_{\mathbf{k}i}(\mathbf{r})$$

does not change the result. This is crucial for implementation, as the phase of eigenvectors is arbitrary, chosen by the diagonalization routine.

We check the gauge invariance by

$$\frac{\partial}{\partial k_\nu}\widetilde{\psi}_{\mathbf{k}i}(\mathbf{r}) = e^{i\beta_i(\mathbf{k})}(i\beta_i(\mathbf{k})+\frac{\partial}{\partial k_\nu})\psi_{\mathbf{k}i}(\mathbf{r}) \tag{7}$$

which means

$$\frac{1}{2}M^{\mathcal{B}}_{\mu\nu}(\mathbf{k}) = \sum_{i,j\in\mathcal{B}}\langle\frac{\partial}{\partial k_\mu}\widetilde{\psi}_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\widetilde{\psi}_{\mathbf{k}j}\rangle\langle\widetilde{\psi}_{\mathbf{k}j}|)|\frac{\partial}{\partial k_\nu}\widetilde{\psi}_{\mathbf{k}i}\rangle = \tag{8}$$

$$\langle(i\beta_i(\mathbf{k})+\frac{\partial}{\partial k_\mu})\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|(i\beta_i(\mathbf{k})+\frac{\partial}{\partial k_\nu})\psi_{\mathbf{k}i}\rangle = \tag{9}$$

$$= \langle\frac{\partial}{\partial k_\mu}\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\frac{\partial}{\partial k_\nu}\psi_{\mathbf{k}i}\rangle \tag{10}$$

$$+(-i\beta_i(\mathbf{k}))(i\beta_i(\mathbf{k}))\langle\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\psi_{\mathbf{k}i}\rangle \tag{11}$$

$$-i\beta_i(\mathbf{k})\langle\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\frac{\partial}{\partial k_\nu}\psi_{\mathbf{k}i}\rangle \tag{12}$$

$$+i\beta_i(\mathbf{k})\langle\frac{\partial}{\partial k_\mu}\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\psi_{\mathbf{k}i}\rangle \tag{13}$$

The last three terms vanish because

$$\langle\phi|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\psi_{\mathbf{k}i}\rangle = \langle\phi|\psi_{\mathbf{k}i}\rangle - \langle\phi|\psi_{\mathbf{k}i}\rangle\langle\psi_{\mathbf{k}i}|\psi_{\mathbf{k}i}\rangle = 0$$

This shows that we could use periodic part of the Bloch functions $u_{\mathbf{k}i}(\mathbf{r})$ instead of $\psi_{\mathbf{k}i}(\mathbf{r}) = e^{i\mathbf{k}\mathbf{r}}u_{\mathbf{k}i}(\mathbf{r})$. This is crucial when we take finite differences, because $\langle\psi_{\mathbf{k}i}|\psi_{\mathbf{k}+\mathbf{q},i}\rangle = 0$ unless $\mathbf{q}=0$, while $\langle u_{\mathbf{k}i}|u_{\mathbf{k}+\mathbf{q},i}\rangle \neq 0$.

Next we choose a finite difference approximation for the derivatives, and produce the formula

$$\frac{1}{2}M^{\mathcal{B}}_{\mu\nu}(\mathbf{k}) = \frac{1}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\langle u_{\mathbf{k}+\Delta_\mu,i} - u_{\mathbf{k},i}|(1-\sum_{j\in\mathcal{B}}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|)|u_{\mathbf{k}+\Delta_\nu i} - u_{\mathbf{k},i}\rangle \tag{14}$$

$$= \frac{1}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\langle u_{\mathbf{k}+\Delta_\mu,i}|(1-\sum_{j\in\mathcal{B}}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|)|u_{\mathbf{k}+\Delta_\nu i}\rangle \tag{15}$$

Note that the rest of the terms generated by the above formula all vanish for the same reason as we shown above. The terms are:

$$-\frac{1}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\langle u_{\mathbf{k}+\Delta_\mu,i}|(1-\sum_{j\in\mathcal{B}}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|)|u_{\mathbf{k},i}\rangle = 0 \tag{16}$$

$$-\frac{1}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\langle u_{\mathbf{k},i}|(1-\sum_{j\in\mathcal{B}}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|)|u_{\mathbf{k}+\Delta_\nu i}\rangle = 0 \tag{17}$$

$$+\frac{1}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\langle u_{\mathbf{k},i}|(1-\sum_{j\in\mathcal{B}}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|)|u_{\mathbf{k},i}\rangle = 0 \tag{18}$$

In cartesian coordinates $\Delta_1 = \Delta\vec{e}_x$, the above formula takes the form

$$\frac{1}{2}M^{\mathcal{B}}_{\mu\mu}(\mathbf{k}) = \frac{1}{\Delta_\mu\Delta_\mu}\sum_{i\in\mathcal{B}}\left(1-\sum_{j\in\mathcal{B}}|\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}j}\rangle|^2\right) \tag{19}$$

and hence the diagonal components of the quantum geometric tensor are:

$$g_{\mu\mu}(\mathbf{k}) = \frac{2}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\left(1-\sum_{j\in\mathcal{B}}|\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}j}\rangle|^2\right) \tag{20}$$

The off diagonal terms are

$$g_{\mu\nu}(\mathbf{k}) = \frac{1}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\left(\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}+\Delta_\nu,i}\rangle + \langle u_{\mathbf{k}+\Delta_\nu,i}|u_{\mathbf{k}+\Delta_\mu,i}\rangle - \sum_{j\in\mathcal{B}}(\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|u_{\mathbf{k}+\Delta_\nu,i}\rangle + \langle u_{\mathbf{k}+\Delta_\nu,i}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|u_{\mathbf{k}+\Delta_\mu,i}\rangle)\right) \tag{21}$$

or

$$g_{\mu\nu}(\mathbf{k}) = \frac{2}{\Delta_\mu\Delta_\nu}\sum_{i\in\mathcal{B}}\mathrm{Re}\left(\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}+\Delta_\nu,i}\rangle - \sum_{j\in\mathcal{B}}\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|u_{\mathbf{k}+\Delta_\nu,i}\rangle\right) \tag{22}$$

For degeneracies at momentum point $\mathbf{k}$ and some set of bands, an arbitrary unitary transformation between these bands should not change the result.

$$|\widetilde{u}_{\mathbf{k}i}\rangle = \sum_{i'\in dg} U_{ii'}(\mathbf{k})\,|u_{\mathbf{k}i'}\rangle$$

To make the formula for $g_{\mu\nu}$ invariant, we need to enlarge the space of $\mathcal{B}$, so that it contains all degenerate bands. For the diagonal components, it is easy to show that the formula is invariant

$$g_{\mu\mu}(\mathbf{k}) = \frac{2}{\Delta_\mu\Delta_\mu}\sum_{i'\in\mathcal{B}}\left(1-\sum_{jj'j''i'i''\in\mathcal{B}} U_{jj'}(\mathbf{k})U^*_{jj''}(\mathbf{k})U^*_{ii'}(\mathbf{k}+\Delta_\mu)U_{ii''}(\mathbf{k}+\Delta_\mu)\langle u_{\mathbf{k}+\Delta_\mu,i'}|u_{\mathbf{k}j'}\rangle\langle u_{\mathbf{k}j''}|u_{\mathbf{k}+\Delta_\mu,i''}\rangle\right) \tag{23}$$

For off-diagonals we have

$$g_{\mu\nu}(\mathbf{k}) = \frac{2}{\Delta_\mu\Delta_\nu}\sum_{i,i',i''\in\mathcal{B}}\mathrm{Re}\left(U^*_{ii'}(\mathbf{k}+\Delta_\mu)U_{ii''}(\mathbf{k}+\Delta_\nu)\left(\langle u_{\mathbf{k}+\Delta_\mu,i'}|u_{\mathbf{k}+\Delta_\nu,i''}\rangle\right.\right. \tag{24}$$

$$\left.\left. - \sum_{j,j',j''\in\mathcal{B}} U^*_{j,j''}(\mathbf{k})U_{jj'}(\mathbf{k})\langle u_{\mathbf{k}+\Delta_\mu,i'}|u_{\mathbf{k}j'}\rangle\langle u_{\mathbf{k}j''}|u_{\mathbf{k}+\Delta_\nu,i''}\rangle\right)\right) \tag{25}$$

The diagonal is clearly invariant, because $U^\dagger U = 1$. The off diagonal terms are not, because we have

$$(U^\dagger(\mathbf{k}+\Delta_\mu)U(\mathbf{k}+\Delta_\nu))_{i'i''}$$

and unitary transformation at different points are not related. This issue arrises because of our finite difference formula, showing that not every implementation is guaranteed to work numerically.

The solution is to use symmetrized formula, which is gauge invariant. We start by writing the symmetrized formula using projectors:

$$g_{\mu\nu}(\mathbf{k}) = \sum_{ij\in\mathcal{B}} \mathrm{Tr}\left(\partial_\mu P_i(\mathbf{k})\partial_\nu P_j(\mathbf{k})\right) \tag{26}$$

where projector is

$$P_i(\mathbf{k}) = |\psi_{\mathbf{k}i}\rangle\langle\psi_{\mathbf{k}i}|$$

We will first show that this formula is equivalent to above given formula in the limit where finite difference is turned into a derivative. After that, we will discretize this formula, and show that it is invariant to any unitary transformation of gauge. We start by rewriting Eq. 26 into something more commonly used for quantum metric tensor:

$$\begin{aligned}
g_{\mu\nu}(\mathbf{k}) &= \sum_{ij\in\mathcal{B}} \mathrm{Tr}\left(\partial_\mu P_i(\mathbf{k})\partial_\nu P_j(\mathbf{k})\right) \\
&\sum_{ij\in\mathcal{B}} \mathrm{Tr}\left(\left(|\partial_\mu\psi_{\mathbf{k}i}\rangle\langle\psi_{\mathbf{k}i}| + |\psi_{\mathbf{k}i}\rangle\langle\partial_\mu\psi_{\mathbf{k}i}|\right)\left(|\partial_\nu\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}| + |\psi_{\mathbf{k}j}\rangle\langle\partial_\nu\psi_{\mathbf{k}j}|\right)\right) \\
&= \sum_{ij\in\mathcal{B}} \mathrm{Tr}\left(|\partial_\mu\psi_{\mathbf{k}i}\rangle\langle\psi_{\mathbf{k}i}|\partial_\nu\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}| + |\partial_\mu\psi_{\mathbf{k}i}\rangle\langle\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle\langle\partial_\nu\psi_{\mathbf{k}j}| + |\psi_{\mathbf{k}i}\rangle\langle\partial_\mu\psi_{\mathbf{k}i}|\partial_\nu\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}| + |\psi_{\mathbf{k}i}\rangle\langle\partial_\mu\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle\langle\partial_\nu\psi_{\mathbf{k}j}|\right) \\
&= \sum_{ij\in\mathcal{B}} \mathrm{Tr}\left(\langle\psi_{\mathbf{k}i}|\partial_\nu\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|\partial_\mu\psi_{\mathbf{k}i}\rangle + \langle\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle\langle\partial_\nu\psi_{\mathbf{k}j}|\partial_\mu\psi_{\mathbf{k}i}\rangle + \langle\partial_\mu\psi_{\mathbf{k}i}|\partial_\nu\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|\psi_{\mathbf{k}i}\rangle + \langle\partial_\mu\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle\langle\partial_\nu\psi_{\mathbf{k}j}|\psi_{\mathbf{k}i}\rangle\right) \\
&= \sum_{ij\in\mathcal{B}} \left(\delta_{ij}(\langle\partial_\nu\psi_{\mathbf{k}j}|\partial_\mu\psi_{\mathbf{k}i}\rangle + \langle\partial_\mu\psi_{\mathbf{k}i}|\partial_\nu\psi_{\mathbf{k}j}\rangle) + \langle\psi_{\mathbf{k}i}|\partial_\nu\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|\partial_\mu\psi_{\mathbf{k}i}\rangle + \langle\partial_\mu\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle\langle\partial_\nu\psi_{\mathbf{k}j}|\psi_{\mathbf{k}i}\rangle\right)
\end{aligned} \tag{27}$$

Because $\partial_\mu(\langle\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle) = 0$ we have $\langle\partial_\mu\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle = -\langle\psi_{\mathbf{k}i}|\partial_\mu\psi_{\mathbf{k}j}\rangle$ hence the last line is

$$g_{\mu\nu}(\mathbf{k}) = \sum_{i\in\mathcal{B}} \langle\partial_\nu\psi_{\mathbf{k}i}|\partial_\mu\psi_{\mathbf{k}i}\rangle + \langle\partial_\mu\psi_{\mathbf{k}i}|\partial_\nu\psi_{\mathbf{k}i}\rangle - \sum_{ij\in\mathcal{B}} \langle\partial_\nu\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|\partial_\mu\psi_{\mathbf{k}i}\rangle - \langle\partial_\mu\psi_{\mathbf{k}i}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|\partial_\nu\psi_{\mathbf{k}i}\rangle \tag{28}$$

$$= \sum_{i\in\mathcal{B}} \langle\partial_\nu\psi_{\mathbf{k}i}|\left(1 - \sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|\right)|\partial_\mu\psi_{\mathbf{k}i}\rangle + \langle\partial_\mu\psi_{\mathbf{k}i}|\left(1 - \sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|\right)|\partial_\nu\psi_{\mathbf{k}i}\rangle \tag{29}$$

which concludes the proof that $g_{\mu\nu}$ with projectors is equivalent to original definition.

Next we discretize the formula 26:

$$g_{\mu\nu}(\mathbf{k}) = \frac{1}{\Delta_\nu\Delta_\mu}\sum_{ij\in\mathcal{B}} \mathrm{Tr}\left(\left(|u_{\mathbf{k}+\Delta_\mu,i}\rangle\langle u_{\mathbf{k}+\Delta_\mu,i}| - |u_{\mathbf{k}i}\rangle\langle u_{\mathbf{k}i}|\right)\left(|u_{\mathbf{k}+\Delta_\nu,j}\rangle\langle u_{\mathbf{k}+\Delta_\nu,j}| - |u_{\mathbf{k}j}\rangle\langle u_{\mathbf{k}j}|\right)\right) \tag{30}$$

$$= \frac{1}{\Delta_\nu\Delta_\mu}\sum_{ij\in\mathcal{B}} \delta_{ij} + |\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}+\Delta_\nu,j}\rangle|^2 - |\langle u_{\mathbf{k}+\Delta_\nu,j}|u_{\mathbf{k}i}\rangle|^2 - |\langle u_{\mathbf{k}+\Delta_\mu,i}|u_{\mathbf{k}j}\rangle|^2 \tag{31}$$

This last equation is clearly gauge invariant, because it only contains absolute values squared. The diagonal part is equal to the above derived Eq. 20

$$g_{\mu\mu}(\mathbf{k}) = \frac{2}{\Delta_\mu\Delta_\mu}\sum_{ij\in\mathcal{B}} \delta_{ij} - |\langle u_{\mathbf{k}+\Delta_\mu,j}|u_{\mathbf{k}i}\rangle|^2. \tag{32}$$

The advantage of this formula is of course that off-diagonal components can be safely computed numerically.

It is convenient to project $g_{\mu\mu}$ to a band, and we define $g^i_{\mu\mu}(\mathbf{k})$ such that $g_{\mu\mu} = \sum_{i\in\mathcal{B}} g^i_{\mu\mu}$. We also symmetrize with respect to the positive and the negative directions, to obtain

$$g^j_{\mu\mu}(\mathbf{k}) = \frac{1}{(\Delta_\mu)^2}\left(1 - \sum_{i\in\mathcal{B}}|\langle u_{\mathbf{k}+\Delta_\mu,j}|u_{\mathbf{k}i}\rangle|^2 + 1 - \sum_{i\in\mathcal{B}}|\langle u_{\mathbf{k}-\Delta_\mu,j}|u_{\mathbf{k}i}\rangle|^2\right). \tag{33}$$

A. Regularization

It turns out that $g_{\mu\nu}(\mathbf{k})$ is often diverging when two bands almost touch. However, such divergence does not contribute to the superfluid weight. The equation for superfluid weight contains factors that cancel such divergence, which however vanish in the limit of large gap. For general case with crossing bands it is more appropriately to not take the limit of large gap, hence we will go back to Eq.20 in PRB 95, 024515 (2017). It shows that

$$\begin{aligned} D^{\mu\nu}_{geom} &= \sum_{\mathbf{k},m\neq n} \Delta^2 \left[\frac{\tanh(\beta/2\sqrt{\varepsilon_m^2+\Delta^2})}{\sqrt{\varepsilon_m^2+\Delta^2}} - \frac{\tanh(\beta/2\sqrt{\varepsilon_n^2+\Delta^2})}{\sqrt{\varepsilon_n^2+\Delta^2}} \right] \\ &\times \frac{\varepsilon_n-\varepsilon_m}{\varepsilon_n+\varepsilon_m} \left[\langle \partial_\nu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \langle \psi_{\mathbf{k}n} | \partial_\mu \psi_{\mathbf{k}m} \rangle + \langle \partial_\mu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \langle \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle \right] \end{aligned} \tag{34}$$

Here energies are measured from the Fermi level.

We will adopt the second line in this expression as the modified metric tensor, i.e.,

$$\widetilde{g}_{\mu\nu} = \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_n-\varepsilon_m}{\varepsilon_n+\varepsilon_m} \left[\langle \partial_\nu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \langle \psi_{\mathbf{k}n} | \partial_\mu \psi_{\mathbf{k}m} \rangle + \langle \partial_\mu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \langle \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle \right] \tag{35}$$

Clearly, in the limit of large gap between the bands in $\mathcal{B}$ and those outside $\mathcal{B}$, it must be that the ratio of energies approaches $\frac{\varepsilon_n-\varepsilon_m}{\varepsilon_n+\varepsilon_m} \to 1$, because ε_m remains small (in the gap), and ε_n is of the order of the gap.

Next we prove that the gauge invariant formula has similar form to the one used before, namely,

$$\widetilde{g}_{\mu\nu} = \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_m-\varepsilon_n}{\varepsilon_m+\varepsilon_n} \mathrm{Tr}\left[\partial_\mu(|\psi_{\mathbf{k}n}\rangle \langle \psi_{\mathbf{k}n}|) \partial_\nu(|\psi_{\mathbf{k}m}\rangle \langle \psi_{\mathbf{k}m}|) \right] \tag{36}$$

The proof goes in the same way as in Eq. 27, the only difference being that sums over n, m are different than before, and therefore $\delta_{n,m}$ here vanishes. But let us repeat the proof:

$$\begin{aligned} \widetilde{g}_{\mu\nu} &= \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_m-\varepsilon_n}{\varepsilon_m+\varepsilon_n} \mathrm{Tr}\left[\partial_\mu(|\psi_{\mathbf{k}n}\rangle \langle \psi_{\mathbf{k}n}|) \partial_\nu(|\psi_{\mathbf{k}m}\rangle \langle \psi_{\mathbf{k}m}|) \right] \qquad (37) \\ &= \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_m-\varepsilon_n}{\varepsilon_m+\varepsilon_n} \mathrm{Tr}\left[(|\partial_\mu\psi_{\mathbf{k}n}\rangle \langle \psi_{\mathbf{k}n}| + |\psi_{\mathbf{k}n}\rangle \langle \partial_\mu\psi_{\mathbf{k}n}|)(|\partial_\nu\psi_{\mathbf{k}m}\rangle \langle \psi_{\mathbf{k}m}| + |\psi_{\mathbf{k}m}\rangle \langle \partial_\nu\psi_{\mathbf{k}m}|) \right] \\ &= \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_m-\varepsilon_n}{\varepsilon_m+\varepsilon_n} \left[\langle \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle \langle \psi_{\mathbf{k}m} | \partial_\mu \psi_{\mathbf{k}n} \rangle + \langle \partial_\mu \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle \delta_{nm} + \delta_{nm} \langle \partial_\nu \psi_{\mathbf{k}m} | \partial_\mu \psi_{\mathbf{k}n} \rangle + \langle \partial_\mu \psi_{\mathbf{k}n} | \psi_{\mathbf{k}m} \rangle \langle \partial_\nu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \right] \end{aligned}$$

Because $m \in \mathcal{B}$ and $n \notin \mathcal{B}$ we can drop the middle two terms containing δ_{nm}. We also use $\langle \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle = -\langle \partial_\nu \psi_{\mathbf{k}n} | \psi_{\mathbf{k}m} \rangle$ because $\partial_\nu \langle \psi_{\mathbf{k}n} | \psi_{\mathbf{k}m} \rangle = 0$. We thus have

$$\begin{aligned} \widetilde{g}_{\mu\nu} &= \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_m-\varepsilon_n}{\varepsilon_m+\varepsilon_n} \left[\langle \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle \langle \psi_{\mathbf{k}m} | \partial_\mu \psi_{\mathbf{k}n} \rangle + \langle \partial_\mu \psi_{\mathbf{k}n} | \psi_{\mathbf{k}m} \rangle \langle \partial_\nu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \right] \\ &= -\sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_m-\varepsilon_n}{\varepsilon_m+\varepsilon_n} \left[\langle \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle \langle \partial_\mu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle + \langle \psi_{\mathbf{k}n} | \partial_\mu \psi_{\mathbf{k}m} \rangle \langle \partial_\nu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \right] \\ &= \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_n-\varepsilon_m}{\varepsilon_m+\varepsilon_n} \left[\langle \partial_\mu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \langle \psi_{\mathbf{k}n} | \partial_\nu \psi_{\mathbf{k}m} \rangle + \langle \partial_\nu \psi_{\mathbf{k}m} | \psi_{\mathbf{k}n} \rangle \langle \psi_{\mathbf{k}n} | \partial_\mu \psi_{\mathbf{k}m} \rangle \right] \end{aligned} \tag{38}$$

which concludes the proof.

The finite difference formula for $\widetilde{g}_{\mu\nu}$ is

$$\begin{aligned} \widetilde{g}_{\mu\nu} &= \frac{1}{\Delta_\mu\Delta_\nu} \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_m-\varepsilon_n}{\varepsilon_m+\varepsilon_n} \mathrm{Tr}\left[(|u_{n,\mathbf{k}+\Delta_\mu}\rangle \langle u_{n,\mathbf{k}+\Delta_\mu}| - |u_{n,\mathbf{k}}\rangle \langle u_{n,\mathbf{k}}|)(|u_{m,\mathbf{k}+\Delta_\nu}\rangle \langle u_{m,\mathbf{k}+\Delta_\nu}| - |u_{m,\mathbf{k}}\rangle \langle u_{m,\mathbf{k}}|) \right] \\ &= \frac{1}{\Delta_\mu\Delta_\nu} \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_n-\varepsilon_m}{\varepsilon_n+\varepsilon_m} \left[|\langle u_{m,\mathbf{k}+\Delta_\nu} | u_{n,\mathbf{k}} \rangle|^2 + |\langle u_{n,\mathbf{k}+\Delta_\mu} | u_{m,\mathbf{k}} \rangle|^2 - |\langle u_{n,\mathbf{k}+\Delta_\mu} | u_{m,\mathbf{k}+\Delta_\nu} \rangle|^2 - |\langle u_{n,\mathbf{k}} | u_{m,\mathbf{k}} \rangle|^2 \right] \end{aligned}$$

The diagonal expression is than

$$\widetilde{g}_{\mu\mu} = \frac{1}{\Delta_\mu\Delta_\mu} \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \frac{\varepsilon_n - \varepsilon_m}{\varepsilon_n + \varepsilon_m} \left[|\langle u_{m,\mathbf{k}+\Delta_\mu}|u_{n,\mathbf{k}}\rangle|^2 + |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}}\rangle|^2 \right] \tag{39}$$

We might have problems to converge this numerically, because bands n very far from the Fermi energy might contribute. To avoid that, we should try to use the following formula

$$\widetilde{g}_{\mu\nu} = g_{\mu\nu} + (\widetilde{g}_{\mu\nu} - g_{\mu\nu}) \tag{40}$$

where $(\widetilde{g}_{\mu\nu} - g_{\mu\nu})$ should have small contribution from bands beyond some cutoff energy. We can compute the difference in the following way:

$$\widetilde{g}_{\mu\nu} - g_{\mu\nu} = \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \left(\frac{\varepsilon_m - \varepsilon_n}{\varepsilon_m + \varepsilon_n} - 1 \right) \mathrm{Tr}\left[\partial_\mu(|\psi_{\mathbf{k}n}\rangle\langle\psi_{\mathbf{k}n}|)\partial_\nu(|\psi_{\mathbf{k}m}\rangle\langle\psi_{\mathbf{k}m}|) \right] \tag{41}$$

which can be implemented by

$$\widetilde{g}_{\mu\nu} - g_{\mu\nu} = \frac{1}{\Delta_\mu\Delta_\nu} \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \left(\frac{\varepsilon_n - \varepsilon_m}{\varepsilon_n + \varepsilon_m} - 1 \right) \left[|\langle u_{m,\mathbf{k}+\Delta_\nu}|u_{n,\mathbf{k}}\rangle|^2 + |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}}\rangle|^2 - |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}+\Delta_\nu}\rangle|^2 - |\langle u_{n,\mathbf{k}}|u_{m,\mathbf{k}}\rangle|^2 \right]$$

where the last term is actually always vanishing.

To prove this formula, we will use slightly different derivation. Before we proved the formula

$$g_{\mu\nu} = \sum_{m\in\mathcal{B},n\in\mathcal{B}} \mathrm{Tr}\left[\partial_\mu(|\psi_{\mathbf{k}n}\rangle\langle\psi_{\mathbf{k}n}|)\partial_\nu(|\psi_{\mathbf{k}m}\rangle\langle\psi_{\mathbf{k}m}|) \right] \tag{42}$$

which can also be cast in the following way

$$g_{\mu\nu} = -\sum_{m\in\mathcal{B},n\notin\mathcal{B}} \mathrm{Tr}\left[\partial_\mu(|\psi_{\mathbf{k}n}\rangle\langle\psi_{\mathbf{k}n}|)\partial_\nu(|\psi_{\mathbf{k}m}\rangle\langle\psi_{\mathbf{k}m}|) \right]. \tag{43}$$

This is because

$$0 = \sum_{m\in\mathcal{B}} \mathrm{Tr}\left[\partial_\mu \left(\sum_n |\psi_{\mathbf{k}n}\rangle\langle\psi_{\mathbf{k}n}| \right) \partial_\nu(|\psi_{\mathbf{k}m}\rangle\langle\psi_{\mathbf{k}m}|) \right]. \tag{44}$$

We can than clearly establish that

$$\widetilde{g}_{\mu\nu} - g_{\mu\nu} = \sum_{m\in\mathcal{B},n\notin\mathcal{B}} \left(1 - \frac{\varepsilon_n - \varepsilon_m}{\varepsilon_n + \varepsilon_m} \right) \mathrm{Tr}\left[\partial_\mu(|\psi_{\mathbf{k}n}\rangle\langle\psi_{\mathbf{k}n}|)\partial_\nu(|\psi_{\mathbf{k}m}\rangle\langle\psi_{\mathbf{k}m}|) \right] \tag{45}$$

which has the finite difference formula derived before. This concludes the proof.

Finally, let us repeat all formulas that we will implement:

$$\begin{aligned}
g^m_{\mu\nu} &= \frac{1}{\Delta_\mu\Delta_\nu} \sum_{n\in\mathcal{B}} \left[|\langle u_{n,\mathbf{k}}|u_{m,\mathbf{k}}\rangle|^2 + |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}+\Delta_\nu}\rangle|^2 - |\langle u_{m,\mathbf{k}+\Delta_\nu}|u_{n,\mathbf{k}}\rangle|^2 - |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}}\rangle|^2 \right] \\
\widetilde{g}^m_{\mu\nu} &= \frac{1}{\Delta_\mu\Delta_\nu} \sum_{n\notin\mathcal{B}} \left(\frac{\varepsilon_n - \varepsilon_m}{\varepsilon_n + \varepsilon_m} \right) \left[|\langle u_{m,\mathbf{k}+\Delta_\nu}|u_{n,\mathbf{k}}\rangle|^2 + |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}}\rangle|^2 - |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}+\Delta_\nu}\rangle|^2 - |\langle u_{n,\mathbf{k}}|u_{m,\mathbf{k}}\rangle|^2 \right] \\
\widetilde{g}^m_{\mu\nu} - g^m_{\mu\nu} &= \frac{1}{\Delta_\mu\Delta_\nu} \sum_{n\notin\mathcal{B}} \left(\frac{\varepsilon_n - \varepsilon_m}{\varepsilon_n + \varepsilon_m} - 1 \right) \left[|\langle u_{m,\mathbf{k}+\Delta_\nu}|u_{n,\mathbf{k}}\rangle|^2 + |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}}\rangle|^2 - |\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}+\Delta_\nu}\rangle|^2 - |\langle u_{n,\mathbf{k}}|u_{m,\mathbf{k}}\rangle|^2 \right]
\end{aligned}$$

B. Integral

The integral over the BZ can be defined in the following way:

$$g^{\mathcal{B}}_{\mu\nu} = \frac{1}{2\pi}\int_{BZ} d^3k g_{\mu\nu}(\mathbf{k}) = \frac{(2\pi)^2}{V_{cell}}\int_{BZ}\frac{V_{cell}d^3k}{(2\pi)^3}g_{\mu\nu}(\mathbf{k}) = \frac{(2\pi)^2}{V_{cell}}\frac{1}{N_k}\sum_{\mathbf{k}} g_{\mu\nu}(\mathbf{k}) \tag{46}$$

If the integral is carried over in cartesian coordinates, and Δ_μ and Δ_ν are displacements in cartesian coordinates, the expressions above can be straightforwardly implemented.

However, if we want to use the existing software, which implements the input to Wannier90, we are forced to use derivative in the lattice coordinates and uniform mesh in momentum space. Namely, Wannier90 uses the following matrix elements

$$M^{\mathbf{k},\mathbf{b}}_{mn} = \langle u_{m\mathbf{k}}|u_{n,\mathbf{k}+\mathbf{b}}\rangle \tag{47}$$

where $\mathbf{b}$ is a small vector connecting nearest neighbors, and $\mathbf{k}$ is vector in the first Brillouin zone.

If the integral is carried out in non-orthogonal lattice systems, we need to take into account matric of the lattice coordinates. We have

$$\eta_{ij} = \vec{b}_i\cdot\vec{b}_j = (BR2^T\cdot BR2)_{ij} \tag{48}$$

$$\eta^{ij} = \left(\eta^{-1}\right)_{ij} \tag{49}$$

The gradient is computed as

$$\sum_i \frac{\partial f}{\partial k_i}\vec{e_i} = \sum_{ij}\frac{\partial f}{\partial b_i}\eta^{ij}\vec{b}_j \tag{50}$$

hence

$$M^{\mathcal{B}}_{\mu\nu}(\mathbf{k}) = 2\sum_{i\in\mathcal{B}}\langle\frac{\partial}{\partial k_p}\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\frac{\partial}{\partial k_q}\psi_{\mathbf{k}i}\rangle\,\eta^{pr}\eta^{qt}b^r_\mu b^t_\nu \tag{51}$$

The trace is easier

$$\sum_\mu M^{\mathcal{B}}_{\mu\mu}(\mathbf{k}) = 2\sum_{i\in\mathcal{B}}\langle\frac{\partial}{\partial k_p}\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\frac{\partial}{\partial k_q}\psi_{\mathbf{k}i}\rangle\,\eta^{pr}\eta^{qt}\eta_{tr} \tag{52}$$

$$= 2\sum_{i\in\mathcal{B}}\langle\frac{\partial}{\partial k_p}\psi_{\mathbf{k}i}|(1-\sum_{j\in\mathcal{B}}|\psi_{\mathbf{k}j}\rangle\langle\psi_{\mathbf{k}j}|)|\frac{\partial}{\partial k_q}\psi_{\mathbf{k}i}\rangle\,\eta^{pq} \tag{53}$$

In this way we could reuse Wannier90 projectors $M^{\mathbf{k},\mathbf{b}}_{mn}$. For example, to compute

$$\begin{aligned}\frac{1}{2\pi}\int_{BZ}\sum_p g^{\mathcal{B}}_{pp}(\mathbf{k}) &= \frac{(2\pi)^2}{V_{cell}N_{\mathbf{k}}}\sum_{\mathbf{k},m\in\mathcal{B},n\in\mathcal{B},\nu\mu}\frac{1}{\Delta_\mu\Delta_\nu}\left[\delta_{nm}+|\langle u_{n,\mathbf{k}+\Delta_\mu}|u_{m,\mathbf{k}+\Delta_\nu}\rangle|^2-|\langle u_{n,\mathbf{k}}|u_{m,\mathbf{k}+\Delta_\nu}\rangle|^2-|\langle u_{m,\mathbf{k}}|u_{n,\mathbf{k}+\Delta_\mu}\rangle|^2\right]\eta^{\mu\nu}\\ &= \frac{(2\pi)^2}{V_{cell}N_{\mathbf{k}}}\sum_{\mathbf{k},m\in\mathcal{B},n\in\mathcal{B},\nu,\mu}\frac{1}{\Delta_\mu\Delta_\nu}\left[\delta_{nm}+|M^{\mathbf{k}+\Delta_\mu,\Delta_\nu-\Delta_\mu}_{nm}|^2-|M^{\mathbf{k},\Delta_\nu}_{nm}|^2-|M^{\mathbf{k},\Delta_\mu}_{mn}|^2\right]\eta^{\mu\nu}\end{aligned} \tag{54}$$

1. *Relation to Marzari-Vanderbilt*

The integral of the quantum geometric tensor is equal to the invariant part of the Marzari-Vanderbilt spread functional Ω_I

$$\Omega_I = \frac{V}{(2\pi)^3}\int_{BZ} d^3k\sum_\mu g_{\mu\mu}(\mathbf{k}) \tag{55}$$

where

$$\Omega_I = \sum_n\langle r^2\rangle_n - \sum_{\mathbf{R},m}|\langle\mathbf{R}m|\mathbf{r}|0n\rangle|^2 \tag{56}$$

They also point out that the integral along the path of GQT is a cumulative change of character of a band.

2. Relation to Coulomb interaction

The Coulomb interaction at small $\mathbf{q}$ is also related to geometric tensor. The Coulomb interaction between bands can be written as

$$V_{\mathbf{q}}(\mathbf{k}ij\mathbf{k}'i'j') \equiv \langle\psi_{\mathbf{k}i}\psi^*_{\mathbf{k+q}j}|\frac{e^{i\mathbf{qr}}}{\sqrt{V}}\rangle\,\frac{4\pi}{\mathbf{q}^2}\,\langle\frac{e^{i\mathbf{qr}'}}{\sqrt{V}}|\psi_{\mathbf{k}'i'}\psi^*_{\mathbf{k}'+\mathbf{q}j'}\rangle = \langle u_{\mathbf{k}i}|u_{\mathbf{k+q}j}\rangle\,\frac{4\pi}{\mathbf{q}^2}\,\langle u_{\mathbf{k}'+\mathbf{q}j'}|u_{\mathbf{k}'i'}\rangle \tag{57}$$

The last Eq. is valid as long as $\mathbf{q}$ is in the first BZ. The diagonal part is

$$\sum_{ij\in\mathcal{B}}\frac{4\pi}{\mathbf{q}^2}\delta_{ij} - V_{\mathbf{q}}(\mathbf{k}ij\mathbf{k}ij) = \sum_{ij\in\mathcal{B}}\frac{4\pi}{\mathbf{q}^2}(\delta_{ij} - |\langle u_{\mathbf{k+q}j}|u_{\mathbf{k}i}\rangle|^2) = 2\pi g^{\mathcal{B}}_{\mathbf{qq}}(\mathbf{k}) \tag{58}$$

and is valid only for very small $\mathbf{q}$.

It seems that at small $\mathbf{q}$, we have

$$V_{\mathbf{q}}(\mathbf{k}ii\mathbf{k}ii) = \frac{4\pi}{\mathbf{q}^2} - 2\pi g^{i}_{\mathbf{qq}}(\mathbf{k}) \tag{59}$$

hence the periodic potential modifies the long range Coulomb interaction by exactly the quantum metric. If the lattice is absent, of course we just have the first term. But introduction of the lattice screens the long-range Coulomb interaction of the band i for its quantum metric. Large quantum metric thus reduces log range Coulomb interaction.