Quantum metric and Topology

Tomoki Ozawa
Advanced Institute for Materials Research, Tohoku University, Japan
(Also a Visiting Scientist at RIKEN iTHEMS)

NCTS-iTHEMS Joint Workshop on Matters to Spacetime: Symmetries and Geometry
@ National Center for Theoretical Sciences, Physics Division, National Taiwan University
August 27, 2024

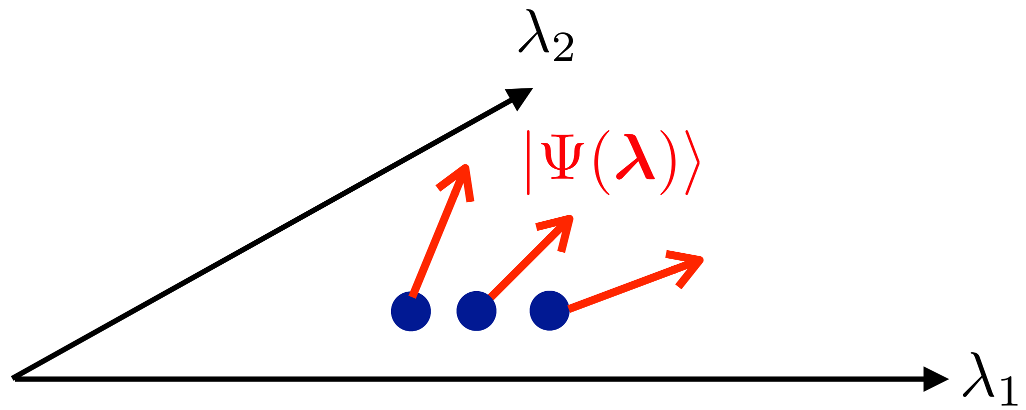
Outline

1. **Definition of the Quantum Metric**
2. Quantum Metric and Topology
3. Quantum Metric and Complex Geometry

Quantum state depending on a set of parameters

Consider a setup where the quantum state $|\Psi(\boldsymbol{\lambda})\rangle$ depends on a set of parameters $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \cdots)$

$\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \cdots)$ can be externally controllable variables, quasi-momentum, or anything



$$|\Psi(\boldsymbol{\lambda})\rangle = \begin{pmatrix} \Psi_1(\boldsymbol{\lambda}) \\ \Psi_2(\boldsymbol{\lambda}) \\ \vdots \\ \Psi_N(\boldsymbol{\lambda}) \end{pmatrix} \in \mathbb{C}^N$$

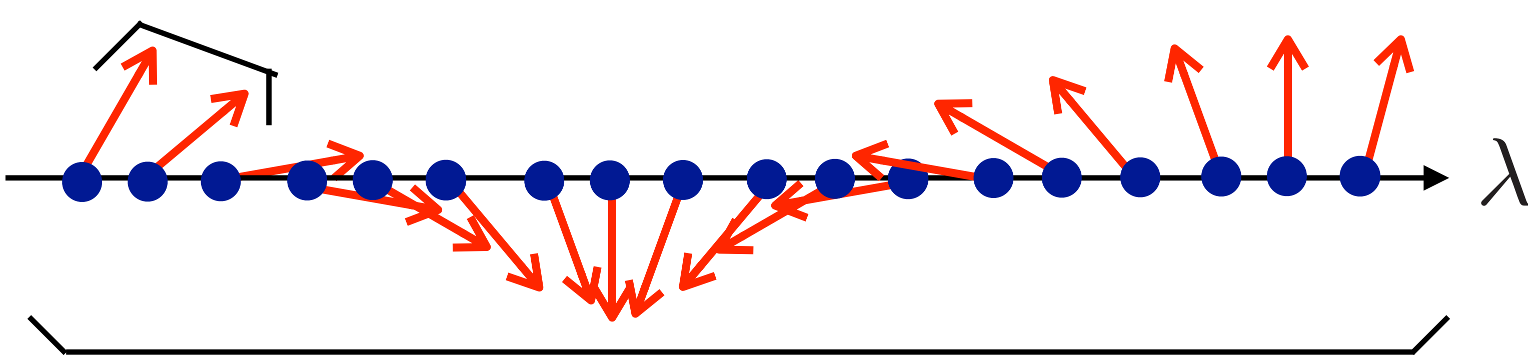
Geometrical property : How much the quantum state changes **locally** in the parameter space

e.g. Berry phase, Berry curvature, quantum metric, etc.

Topological property : How much the quantum state changes **globally** in the parameter space

e.g. Chern number, winding number, Z2 topological invariant, etc.

Geometry: The arrows locally **change their angles**

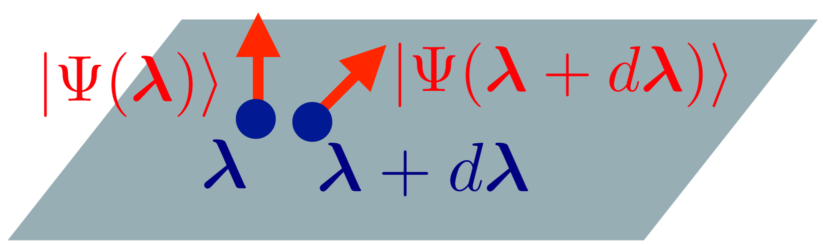


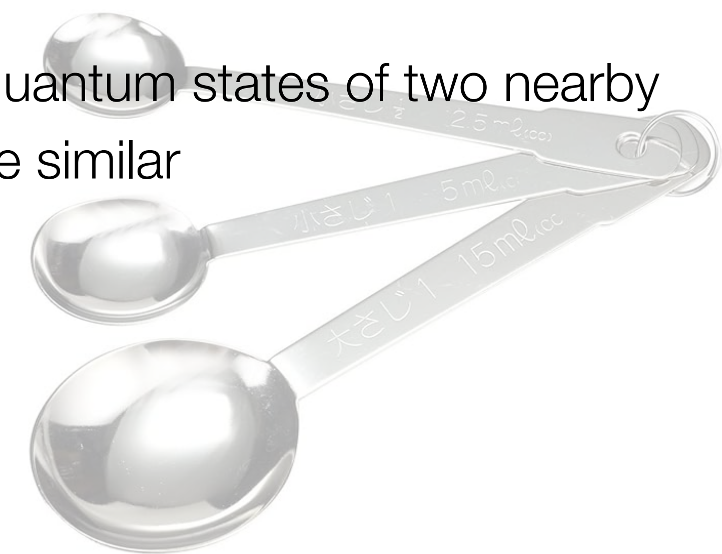
Topology: Overall the arrows **rotate once**

Quantum metric

Metric defines **distance** in the parameter space

Quantum metric is the metric which is defined to assign long distance if quantum states of two nearby points are very different, and assign short distance if the quantum states are similar





Definition of the quantum metric: we define length between infinitesimally close points by the following

$$ds^2 = 1 - |\langle\Psi(\boldsymbol{\lambda}+d\boldsymbol{\lambda})|\Psi(\boldsymbol{\lambda})\rangle|^2 \equiv \sum_{i,j} g_{ij}(\boldsymbol{\lambda}) d\lambda_i d\lambda_j$$

Expanding in Taylor series, one finds the following concrete expression of the quantum metric

$$g_{ij}(\boldsymbol{\lambda}) = \frac{1}{2}\langle\partial_{\lambda_i}\Psi(\boldsymbol{\lambda})|Q(\boldsymbol{\lambda})|\partial_{\lambda_j}\Psi(\boldsymbol{\lambda})\rangle + \frac{1}{2}\langle\partial_{\lambda_j}\Psi(\boldsymbol{\lambda})|Q(\boldsymbol{\lambda})|\partial_{\lambda_i}\Psi(\boldsymbol{\lambda})\rangle$$

$Q(\boldsymbol{\lambda}) \equiv 1 - |\Psi(\boldsymbol{\lambda})\rangle\langle\Psi(\boldsymbol{\lambda})|$: Projection to outside the state $|\Psi(\boldsymbol{\lambda})\rangle$

In this talk, I will focus on the situation where $|\Psi(\boldsymbol{\lambda})\rangle$ is a Bloch state and $\boldsymbol{\lambda} = \mathbf{k} = (k_x, k_y)$ is two-dimensional quasi-momentum space

Bloch state and band structure

Consider a particle moving in a periodic potential $H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r})$ $\quad V(\mathbf{r} + \mathbf{a}_i) = V(\mathbf{r})$

Lattice vector

Eigenstate can be labeled by a band index n and a quasi-momentum **k**

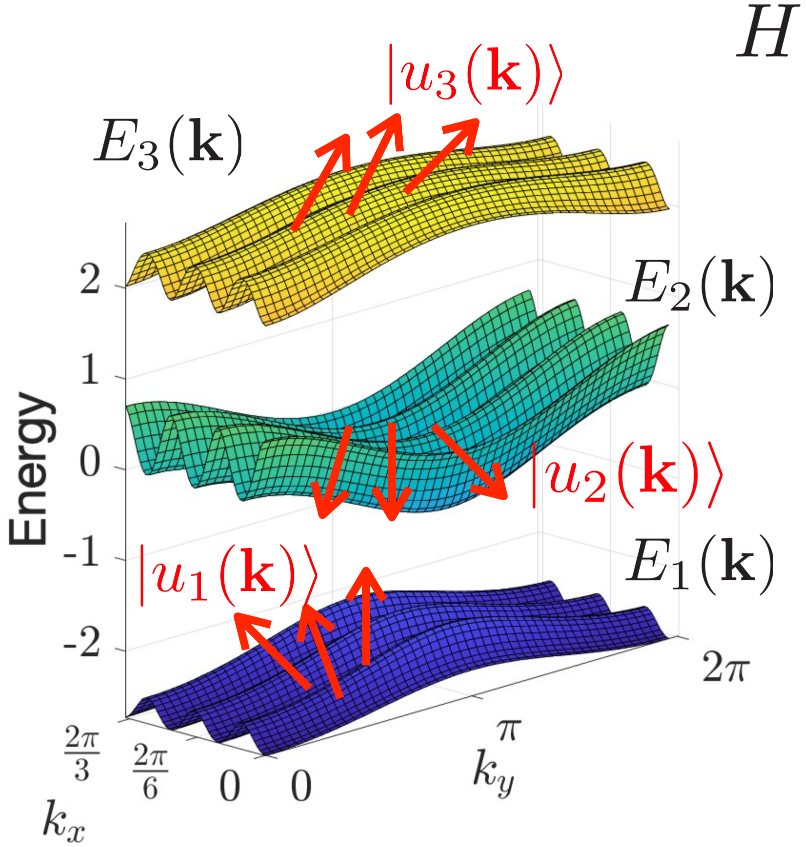
$$H e^{i\mathbf{k}\cdot\mathbf{r}} |u_n(\mathbf{k})\rangle = E_n(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}} |u_n(\mathbf{k})\rangle$$

Cell-periodic part of Bloch state

Bloch state

Or by defining the k-space Hamiltonian $H(\mathbf{k}) \equiv e^{-i\mathbf{k}\cdot\mathbf{r}} H e^{i\mathbf{k}\cdot\mathbf{r}}$, we can write

$$H(\mathbf{k})|u_n(\mathbf{k})\rangle = E_n(\mathbf{k})|u_n(\mathbf{k})\rangle$$



We are interested in the geometrical and topological properties of $|u_n(\mathbf{k})\rangle$ with $\mathbf{k} = (k_x, k_y)$ as a parameter space

In tight-binding setups, $H(\mathbf{k})$ is an N by N Hermitian matrix

Then, $n = 1, 2, \cdots, N$ and

$$|u_n(\mathbf{k})\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

Quantum geometry of Bloch states

From the (cell-periodic part of the) Bloch state, one can define the **quantum geometric tensor**

$$\chi_{ij}(\mathbf{k}) = \langle \partial_{k_i} u_n(\mathbf{k}) | Q(\mathbf{k}) | \partial_{k_j} u_n(\mathbf{k}) \rangle$$

$$Q(\mathbf{k}) \equiv 1 - |u_n(\mathbf{k})\rangle\langle u_n(\mathbf{k})\rangle = \sum_{m\neq n} |u_m(\mathbf{k})\rangle\langle u_m(\mathbf{k})|$$

Projection to the other bands

This quantity is gauge-invariant, i.e. does not depend on how the phase of $|u_n(\mathbf{k})\rangle$ is chosen

Its real part is the **quantum metric:**

$$g_{ij}(\mathbf{k}) = \mathrm{Re}\left[\chi_{ij}(\mathbf{k})\right] = \frac{1}{2}\left(\langle \partial_{k_i} u_n(\mathbf{k}) | Q(\mathbf{k}) | \partial_{k_j} u_n(\mathbf{k}) \rangle + \langle \partial_{k_j} u_n(\mathbf{k}) | Q(\mathbf{k}) | \partial_{k_i} u_n(\mathbf{k}) \rangle\right)$$

Imaginary part is the **Berry curvature:**

$$\Omega_{xy}(\mathbf{k}) = -2\,\mathrm{Im}\left[\chi_{xy}(\mathbf{k})\right] = i\left(\langle \partial_{k_x} u_n(\mathbf{k}) | \partial_{k_y} u_n(\mathbf{k}) \rangle - \langle \partial_{k_y} u_n(\mathbf{k}) | \partial_{k_x} u_n(\mathbf{k}) \rangle\right)$$

Writing the quantum geometric tensor in a matrix form, it looks

$$\chi(\mathbf{k}) = \begin{pmatrix} g_{xx}(\mathbf{k}) & g_{xy}(\mathbf{k}) - i\Omega_{xy}(\mathbf{k})/2 \\ g_{xy}(\mathbf{k}) + i\Omega_{xy}(\mathbf{k})/2 & g_{yy}(\mathbf{k}) \end{pmatrix}$$

Physical appearances of quantum metric

In this talk, I will mainly discuss how the quantum metric is related to **topology in two dimensions**, especially the **Chern number**

However, I should mention that the quantum metric in **momentum space** is known to be related to, or to have consequences in

- **localization** of Wannier functions
- **Optical responses**, which has led to **experimental measurements** of quantum metric in the past couple of years
- **Superfluid density** particularly in the flat band context
- **Semi-classical equations of motion** and **nonlinear response**
- and many more….

Furthermore, in a general parameter space, quantum metric is equivalent to the **quantum Fisher information of pure states** appearing in the **quantum Cramér-Rao bound** in quantum metrology

Outline

1. Definition of the Quantum Metric
2. **Quantum Metric and Topology**
3. Quantum Metric and Complex Geometry

Inequality

Quantum metric and the Berry curvature are real and imaginary parts of the quantum geometric tensor

$$g_{ij}(\mathbf{k}) = \mathrm{Re}\left[\langle \partial_{k_i} u_n(\mathbf{k})|Q(\mathbf{k})|\partial_{k_j} u_n(\mathbf{k})\rangle\right]$$

$$\Omega_{xy}(\mathbf{k}) = -2\,\mathrm{Im}\left[\langle \partial_{k_x} u_n(\mathbf{k})|Q(\mathbf{k})|\partial_{k_y} u_n(\mathbf{k})\rangle\right]$$

Quantum geometric tensor

$$Q(\mathbf{k}) \equiv 1 - |u_n(\mathbf{k})\rangle\langle u_n(\mathbf{k})|$$

Projection to other bands

Since $Q^2 = Q$, by applying the Cauchy-Schwarz inequality, $\langle\alpha|\alpha\rangle\langle\beta|\beta\rangle \geq |\langle\alpha|\beta\rangle|^2$, to $|\alpha\rangle = Q|\partial_{k_x} u_n(\mathbf{k})\rangle,\ |\beta\rangle = Q|\partial_{k_y} u_n(\mathbf{k})\rangle$, one obtains

$$\sqrt{\det g(\mathbf{k})} \geq \frac{|\Omega_{xy}(\mathbf{k})|}{2}$$

Roy, Phys. Rev. B **90**, 165139 (2014)

The equality holds when $\exists c \in \mathbb{C} \quad Q|\partial_{k_x} u_n\rangle = c\,Q|\partial_{k_y} u_n\rangle$

Integrating the both sides of the inequality, we can obtain a global inequality

$$\mathrm{vol}_g \equiv \int_{BZ^2} \sqrt{\det(g(\mathbf{k}))}dk_x dk_y \geq \int_{BZ^2} \frac{|\Omega_{xy}|}{2} dk_x dk_y \geq \left|\int_{BZ^2} \frac{\Omega_{xy}}{2} dk_x dk_y\right| = |\pi\mathcal{C}|$$

(We call it) **quantum volume**

Chern number (topological quantity)

Ozawa & Mera, Phys. Rev. B **104**, 045103 (2021)

Landau levels

Consider a charged particle in a two-dimensional space with a magnetic field

$$H = \frac{1}{2M}\left(-\partial_x^2 + \left(-i\partial_y - Bx\right)^2\right)$$

The quantum metric and the Berry curvature of the lowest level, called the **lowest Landau levels**, is

$$g_{xx}(\mathbf{k}) = g_{yy}(\mathbf{k}) = \frac{1}{4\pi},\ g_{xy}(\mathbf{k}) = 0,\ \Omega_{xy}(\mathbf{k}) = -\frac{1}{2\pi}\mathrm{sign}(B)$$

This is constant in momentums space, and the equality holds:

$$\sqrt{\det(g(\mathbf{k}))} = \frac{|\Omega_{xy}(\mathbf{k})|}{2} = \frac{1}{4\pi}$$

The global equality also holds: $\mathrm{vol}_g = \pi|\mathcal{C}| = \pi$

Landau levels are (energetically and) geometrically flat (uniform) bands
The lowest Landau level is the only geometrically flat band with a unit Chern number satisfying the equality

Ozawa & Mera, Phys. Rev. B **104**, 045103 (2021)

Two-band and multi-band models

Two-band models

Two band models are very special because the following two properties always hold:

- $\sqrt{\det g(\mathbf{k})} = \frac{|\Omega_{xy}(\mathbf{k})|}{2}$ holds everywhere

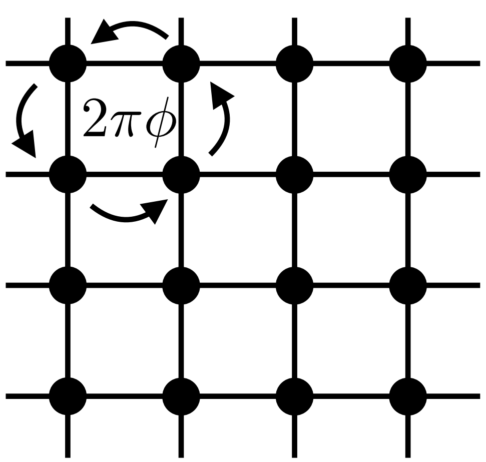
  The equality $\mathrm{vol}_g = \pi|\mathcal{C}|$ holds when the Berry curvature doesn't change sign in momentum space

- There must be points with $\sqrt{\det g(\mathbf{k})} = \frac{|\Omega_{xy}(\mathbf{k})|}{2} = 0$

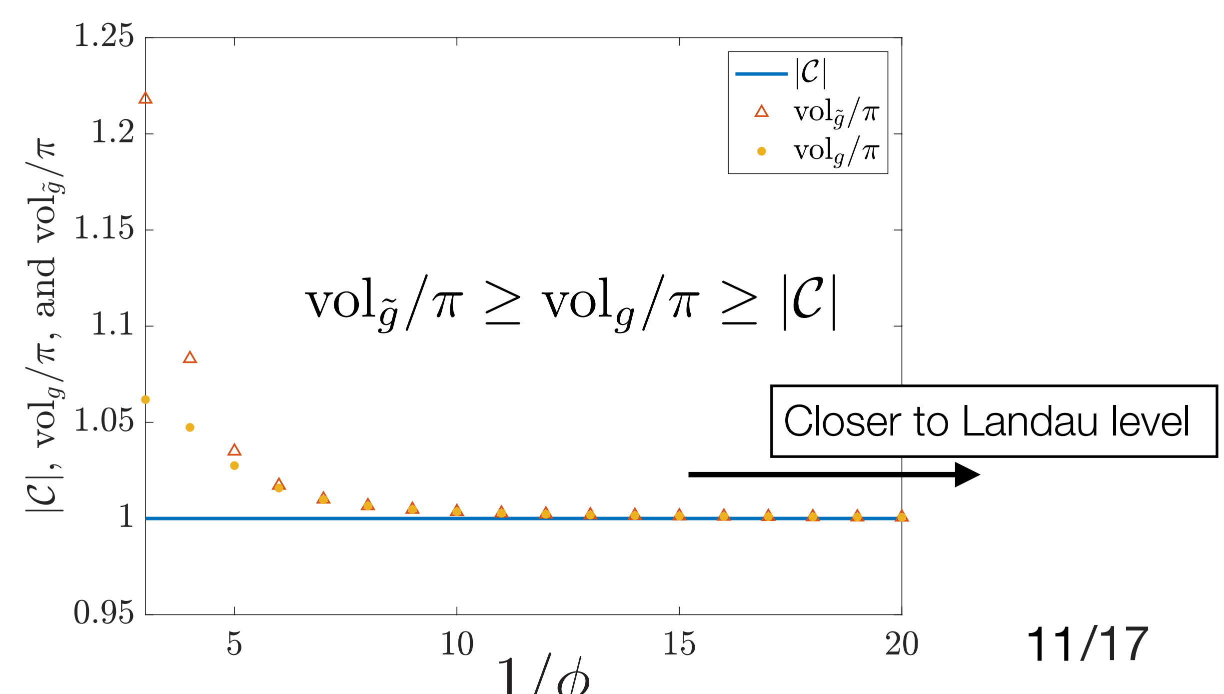
  There must be points in momentum space where the Berry curvature is zero

Multi-band models

Inequality tends to saturate in a limit where bands become flatter or more Landau-level like (very empirical)



$$\sqrt{\det g(\mathbf{k})} \geq \frac{|\Omega_{xy}(\mathbf{k})|}{2}$$



Ozawa & Mera, Phys. Rev. B **104**, 045103 (2021)

Outline

1. Definition of the Quantum Metric
2. Quantum Metric and Topology
3. **Quantum Metric and Complex Geometry**

Quantum states as a map between complex manifolds

Regard the Bloch state as a map from quasi-momentum space to the space of quantum states

Complex projective space

$$u_n : T^2 \longrightarrow \mathbb{C}P^{N-1}$$

Brillouin zone is two-torus

$$\mathbf{k} \longmapsto |u_n(\mathbf{k})\rangle = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_N \end{pmatrix}$$

N: Total number of bands

Complex projective space $\mathbb{C}P^{N-1}$ is a complex manifold (locally described by complex coordinates), and there exists a natural metric known as the Fubini-Study metric g_{FS}

Quantum metric is nothing but the pull-back of the Fubini-Study metric g_{FS} via the Bloch state map
Berry curvature is the pull-back of the symplectic form ω_{FS} naturally defined in $\mathbb{C}P^{N-1}$

Quantum metric: $g = {u_n}^* g_{FS}$ Berry curvature: $\frac{\Omega_{xy}}{2} dk_x \wedge dk_y = {u_n}^* \omega_{FS}$

Complex structure on the Brillouin zone

$$u_n : T^2 \longrightarrow \mathbb{C}P^{N-1}$$

Complex projective space

Brillouin zone is two-torus

We can also look for a **complex structure** (one-dimensional complex coordinate) on the Brillouin zone, which is compatible with the metric, i.e. complex coordinate z which satisfies

$$\sum_{ij} g_{ij} dk_i dk_j \propto |dz|^2$$

When the quantum metric is k-independent, we define the 90 degrees rotation (multiplication by an imaginary unit) on the tangent space by the matrix called the almost complex structure

$$J = \frac{1}{\sqrt{\det g}} \begin{pmatrix} -g_{xy} & -g_{yy} \\ g_{xx} & g_{xy} \end{pmatrix} \equiv \frac{1}{\mathrm{Im}(\tau)} \begin{pmatrix} -\mathrm{Re}(\tau) & -|\tau|^2 \\ 1 & \mathrm{Re}(\tau) \end{pmatrix}$$

which is characterized by a complex number called the modular parameter $\tau = \dfrac{g_{xy} + i\sqrt{\det g}}{g_{xx}} \in \mathbb{H}$

Then, we can define the complex coordinate by $z = k_x + \tau k_y$

Holomorphicity of the map

Regard the Bloch state as a map between complex manifolds (Brillouin zone and $\mathbb{C}P^{N-1}$)

$$u_n : T^2 \longrightarrow \mathbb{C}P^{N-1}$$

Necessary and sufficient condition for the equality $\sqrt{\det g(\mathbf{k})} = \frac{|\Omega_{xy}(\mathbf{k})|}{2}$ to hold everywhere in momentum space is that the map u_n is a **holomorphic map**

Mera & Ozawa, Phys. Rev. B **104**, 045104 (2021), Phys. Rev. B **104**, 115160 (2021)

- The condition is equivalent to the Brillouin zone being a complex manifold called the **Kähler manifold** equipped with quantum metric, Berry curvature, and the complex structure satisfying $g(\mathbf{k}) = \omega(\mathbf{k})J(\mathbf{k})$
- We call the band with equality holding everywhere the **Kähler band**
- **Lowest Landau level** and chiral limit of the flat band of **twisted bilayer graphene** are Kähler bands
- If the complex structure is constant in Brillouin zone, the corresponding Kähler bands are also called **Ideal flatband**, **ideal Chern band**, or **Vortexable band**, and are considered to stabilize fractional quantum Hall states under short-range interactions

Wang, Cano, Millis, Liu, Yang, PRL **127**, 246403 (2021)
Wang and Liu, PRL **128**, 176403 (2022)
Wang, Klevtsov, Liu, PR Research **5**, 023167 (2023)

Ledwith, Vishwanath, Khalaf, PRL **128**, 176404 (2022)
Ledwith, Vishwanath, Parker, arXiv:2209.15023

Uniqueness of the Landau level

Lowest Landau levels are essentially the only Kähler bands with uniform quantum metric & Berry curvature

Theorem

Bloch state with the equality $\sqrt{\det g(\mathbf{k})} = \frac{\Omega_{xy}(\mathbf{k})}{2}$ holding everywhere and quantum metric & Berry curvature are constant in momentum space is unique, once the Chern number and the complex structure (modular parameter $\mathcal{T}$) are given, up to gauge degrees of freedom

Outline of the proof

Map u_n is holomorphic and the complex structure J is constant

→ Bloch state $|u_n(\mathbf{k})\rangle$ must be written as a sum of (holomorphic) theta functions

Furthermore, impose that the quantum metric and the Berry curvature are constant

→ How the sum of the theta functions should be taken is uniquely determined

- When $\mathcal{C} = 1$, the Bloch state is $u_{\mathbf{k}}(x, y) = \vartheta_{-x,y}(k_x + \tau k_y, \tau)$
- When $\mathcal{C} > 1$, $\mathcal{C}$ -component wavefunction with internal degrees of freedom (spin or orbital) is needed

$$u_{\mathbf{k}}(\mathbf{r}) = \begin{pmatrix} \vartheta_{-x/\mathcal{C},y}(\mathcal{C}k_x + \mathcal{C}\tau k_y, \tau) \\ \vartheta_{(1-x)/\mathcal{C},y}(\mathcal{C}k_x + \mathcal{C}\tau k_y, \tau) \\ \vdots \\ \vartheta_{(\mathcal{C}-1-x)/\mathcal{C},y}(\mathcal{C}k_x + \mathcal{C}\tau k_y, \tau) \end{pmatrix}$$

Color-entangled wavefunction

Mera & Ozawa, arXiv:2304.00866 (accepted to Phys. Rev. Research)

Conclusion

- **Quantum metric** is the metric in a parameter space defined from inner product of quantum states
- The **inequality** $\sqrt{\det g(\mathbf{k})} \geq \frac{|\Omega_{xy}(\mathbf{k})|}{2}$ holds between the quantum metric and the Berry curvature
- The **equality** holds for the **lowest Landau level**
- Generally, the equality holds everywhere in momentum space only when the Bloch state is a **holomorphic map** (in an appropriately defined sense), and we call such bands **Kähler bands**
- Kähler bands with constant quantum metric and Berry curvature are the lowest Landau levels and their generalizations to higher Chern numbers and complex structure beyond *i*

The work has been done in collaboration with Bruno Mera from Instituto de Telecomunicações (former Assistant Professor in my group)

References:
Ozawa & Mera, PRB **104**, 045103 (2021)
Mera & Ozawa, PRB **104**, 045104 (2021)
Mera & Ozawa, PRB **104**, 115160 (2021)
Mera & Ozawa, arXiv:2304.00866