Derivation and Characteristics of Geometric Phases in Quantum Mechanics

Introduction to Berry Phase

Tomoaki Kameda 21 June 2024

Review of previous seminar

- Derivation berry phase in general space

Berry phase

Hamiltonian is dependent on some parameter $\boldsymbol{R}$.

we solve time-dependent Schrödinger equation considering adiabatic system.

$$\gamma(t) = i\int_0^t \langle\phi_n(\boldsymbol{R}(t'))|\frac{\partial}{\partial t'}|\phi_n(\boldsymbol{R}(t'))\rangle dt' = i\int_C \langle\phi_n(\boldsymbol{R})|\frac{\partial}{\partial \boldsymbol{R}}|\phi_n(\boldsymbol{R})\rangle\cdot d\boldsymbol{R} = \int_C A_n(\boldsymbol{R})\cdot d\boldsymbol{R}$$

Berry connection $A_n(\boldsymbol{R}) = i\langle\phi_n(\boldsymbol{R})|\frac{\partial}{\partial \boldsymbol{R}}|\phi_n(\boldsymbol{R})\rangle$

Berry curvature $\boldsymbol{B}_n(\boldsymbol{R}) = \nabla_{\boldsymbol{R}}\times\boldsymbol{A}_n(\boldsymbol{R})$

- Expression transformation for numerical calculations

$$B_{n,z}(\boldsymbol{R}) = -2Im\sum_{(m\neq n)}\frac{\langle\phi_n(\boldsymbol{R})|\frac{\partial\hat{H}(\boldsymbol{R})}{\partial R_x}|\phi_m(\boldsymbol{R})\rangle\langle\phi_m(\boldsymbol{R})|\frac{\partial\hat{H}(\boldsymbol{R})}{\partial R_y}|\phi_n(\boldsymbol{R})\rangle}{(E_n-E_m)^2}$$

This formula indicated that we can calculate berry curvature when we get Hamiltonian.

Todays seminar topics

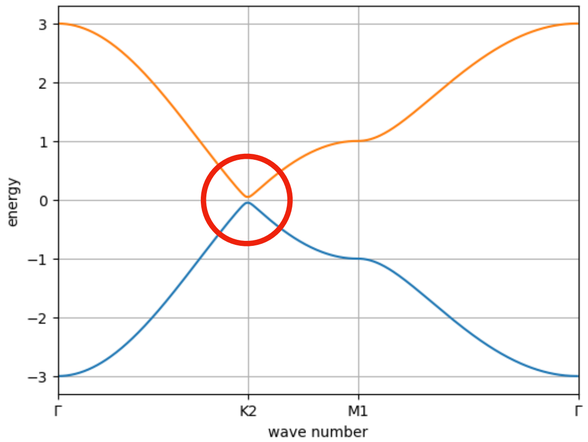
Symmetry and geometric phase, Specific model calculations

- Relationship between symmetry and geometric phase
- Consider Tight binding model about graphene, h-BN and Haldane mode

Berry phase at K point in graphene

Analytical solution

Consider an effective Hamiltonian around the K point.



Graphene band structure

① Expand to first order around K(K′) points with respect to k

$$H_K(\boldsymbol{k}) = \hbar\nu \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} = \hbar(-\sigma_x k_x + \sigma_y k_y).$$

$$\nu = \frac{\sqrt{3}}{2}\frac{a\gamma_0}{\hbar}, \quad \sigma_i (i = x, y, z)$$

$$(k_x, k_y) = k(\cos\phi, \sin\phi)$$

$$|\phi_+(\boldsymbol{k})\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mathrm{e}^{i\phi(\boldsymbol{k})} \end{pmatrix}, \quad |\phi_-(\boldsymbol{k})\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -\mathrm{e}^{i\phi(\boldsymbol{k})} \end{pmatrix}$$

$$\begin{aligned} \mathcal{A}_\pm(\boldsymbol{k}) &= i\,\langle\phi_\pm(\boldsymbol{k})|\nabla_{\boldsymbol{k}}|\phi_\pm(\boldsymbol{k})\rangle \\ &= \frac{1}{2}\nabla_{\boldsymbol{k}}\phi(\boldsymbol{k}), \end{aligned}$$

$$\gamma[C] = \oint \mathcal{A}(\boldsymbol{k}) \cdot d\boldsymbol{k} = \begin{cases} -\pi \\ 0 \end{cases}$$

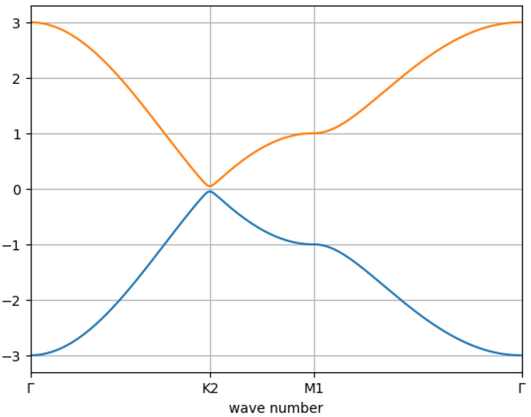
Berry phase in graphene

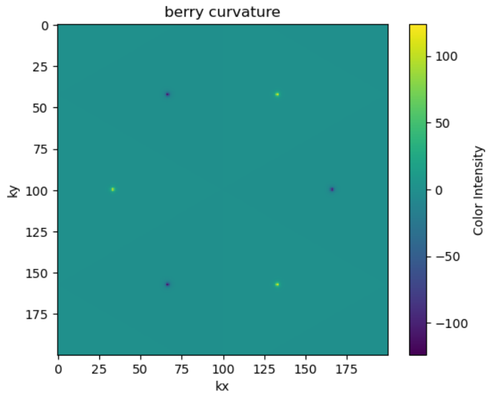
Numerical calculation

Berry curvature

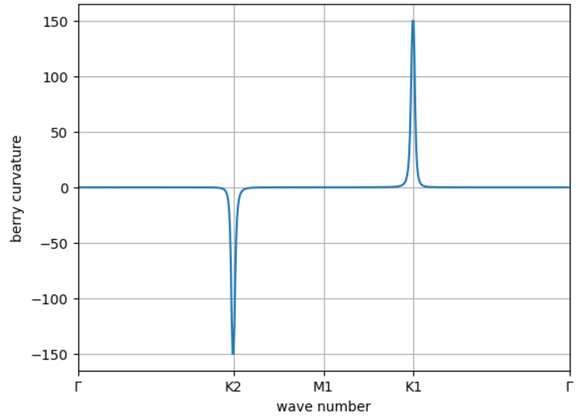
$$B_{n,z}(\boldsymbol{R}) = -2Im \sum_{(m \neq n)} \frac{\langle \phi_n(\boldsymbol{R}) | \frac{\partial \hat{H}(\boldsymbol{R})}{\partial R_x} | \phi_m(\boldsymbol{R}) \rangle \langle \phi_m(\boldsymbol{R}) | \frac{\partial \hat{H}(\boldsymbol{R})}{\partial R_y} | \phi_n(\boldsymbol{R}) \rangle}{(E_n - E_m)^2}$$

High band

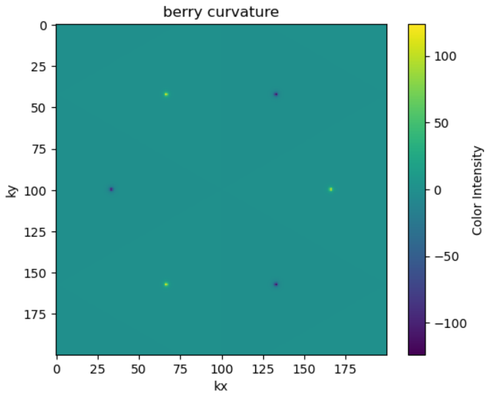




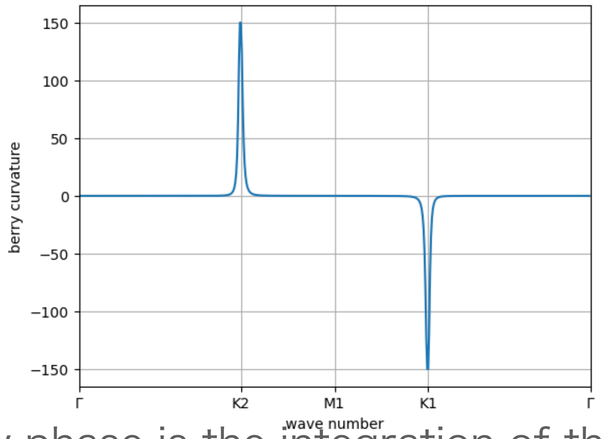
BZ



Low band



BZ



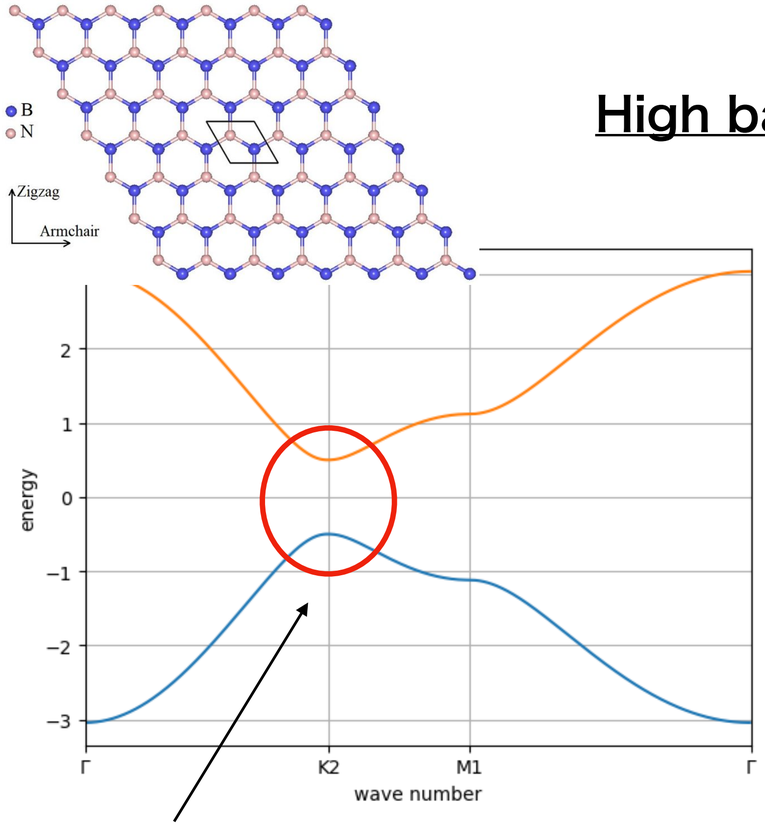
Berry curvature is 0 all over the BZ

but diverges at K(K') point

Berry phase is the integration of the Berry curvature over the entire BZ

Berry phase in h-BN model

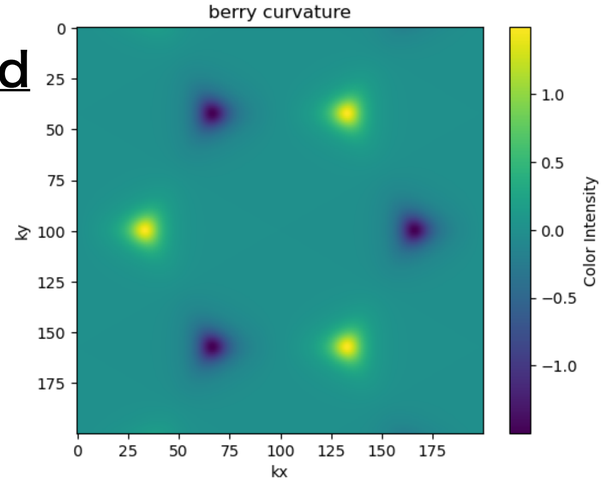
Breaking Inversion symmetry

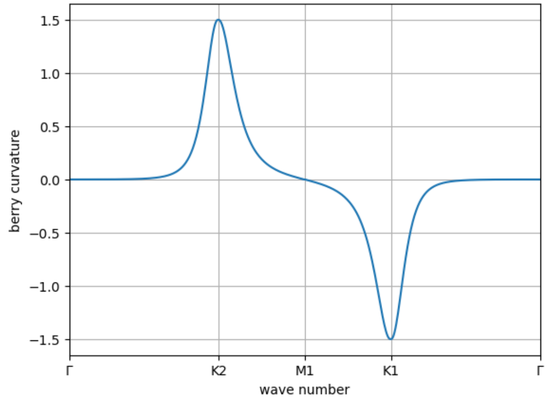


Open energy gap

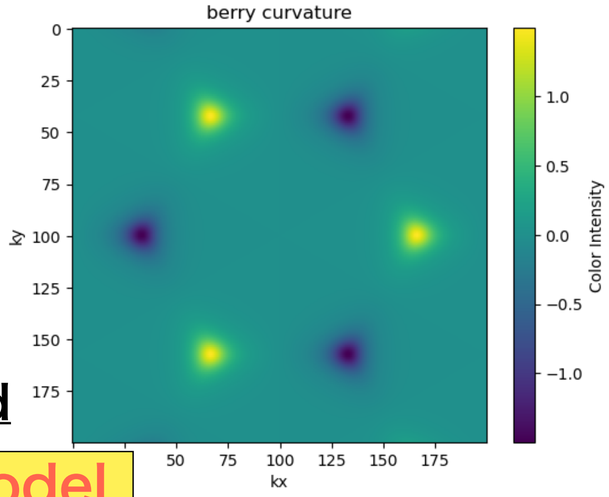
Berry curvature

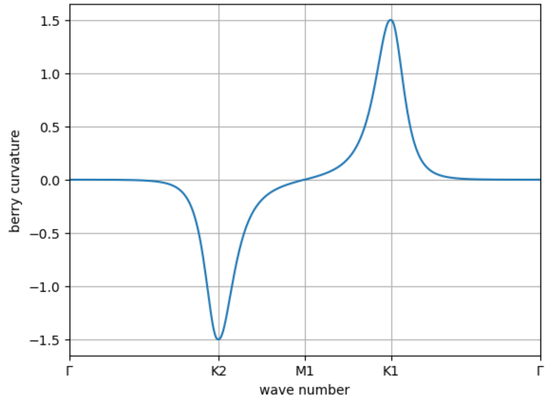
High band





Low band

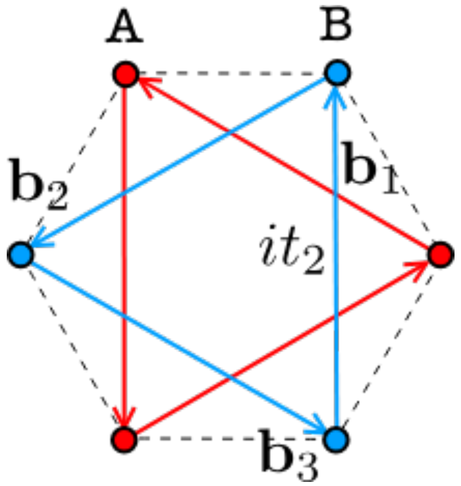


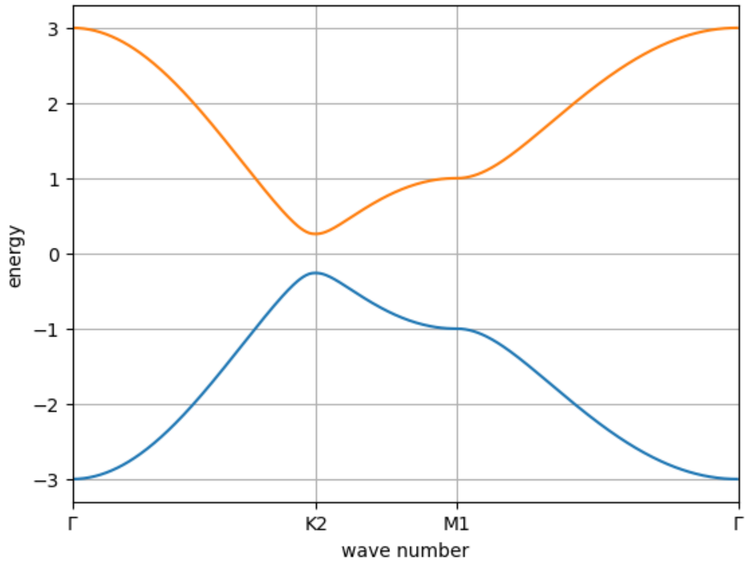


BC is odd-function in h-BN model

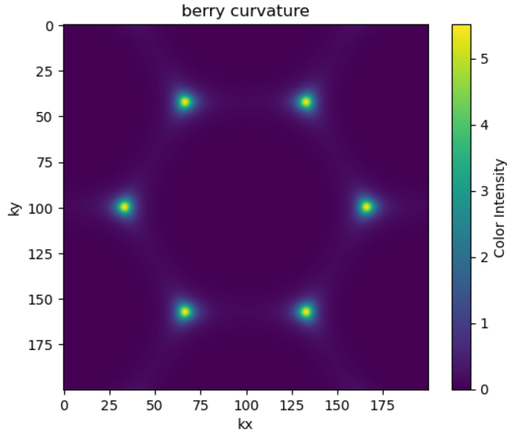
Berry phase in Haldane model

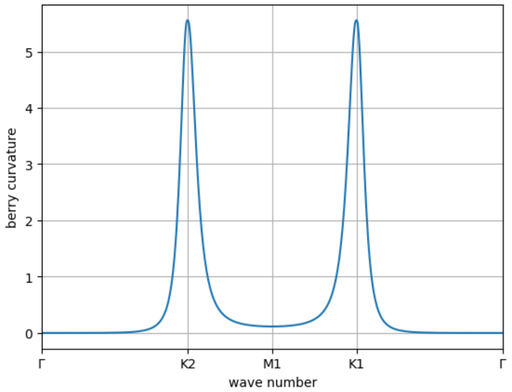
Breaking Time reversal symmetry

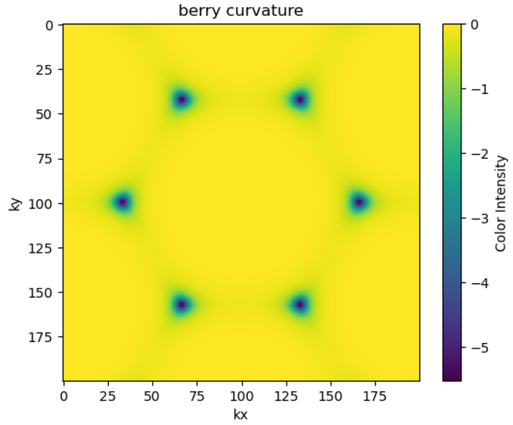


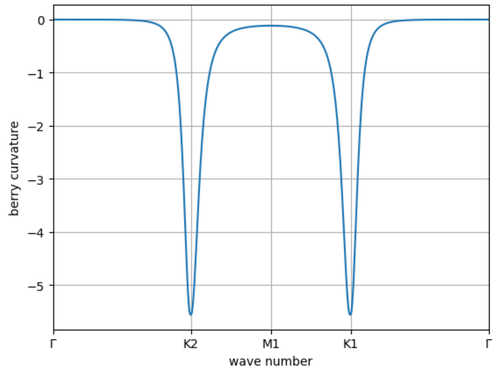


Berry curvature









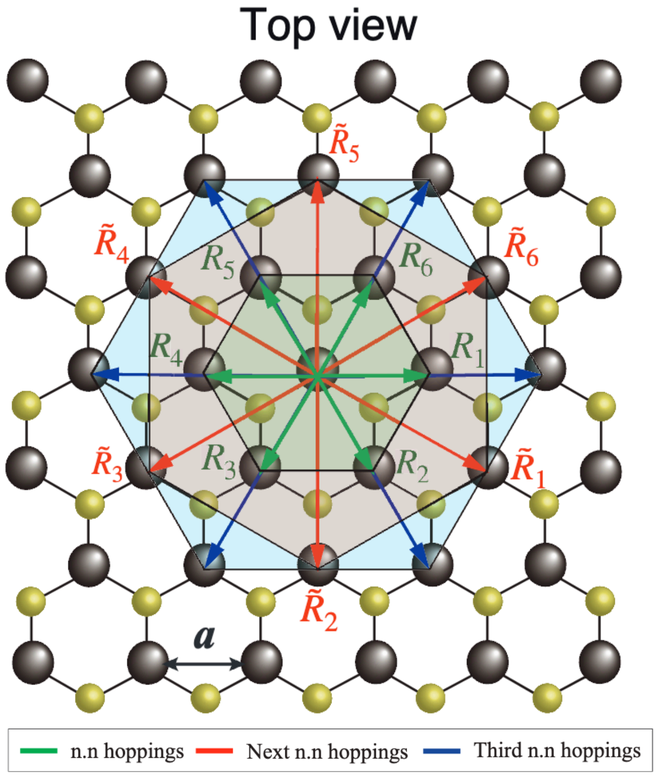
BC is even-function in Haldane model

Progress report

Tomoaki Kameda

Three band tight binding model

Transition metal dichalcogenide structure



Hamiltonian

$$H_{\mathrm{TB}}(\boldsymbol{k}) = \underset{①}{H_{\mathrm{TNN}}(\boldsymbol{k}) \otimes \sigma_0} + \underset{②}{\frac{1}{2}\lambda L_z \otimes \sigma_z} + \underset{③}{H_{\mathrm{R}}(\boldsymbol{k})} + \underset{④}{H_{\mathrm{I}}^{c}(\boldsymbol{k})}$$

① Third nearest neighbor hopping term

② Ising type SOC term (valence band)

③ Rashba type SOC term

Consider about these term

④ Ising type SOC term (conduction band)

$$H_{\mathrm{R}}(\boldsymbol{k}) = \begin{pmatrix} 2\alpha_0 & 0 & 0 \\ 0 & 2\alpha_2 & 0 \\ 0 & 0 & 2\alpha_2 \end{pmatrix} \otimes (f_x(\boldsymbol{k})\sigma_y - f_y(\boldsymbol{k})\sigma_x).$$

Consider 3 band in d orbital of transition atom with spin

$$\left\{ \left| d_{z^2,\uparrow} \right\rangle, \left| d_{xy,\uparrow} \right\rangle, \left| d_{x^2-y^2,\uparrow} \right\rangle, \left| d_{z^2,\downarrow} \right\rangle, \left| d_{xy,\downarrow} \right\rangle, \left| d_{x^2-y^2,\downarrow} \right\rangle \right\}$$

1.Liu, G., Shan, W., Yao, Y., Yao, W. & Xiao, D. Three-band tight-binding model for monolayers of group-VIB transition metal dichalcogenides. *Phys. Rev. B* **88**, 085433 (2013).

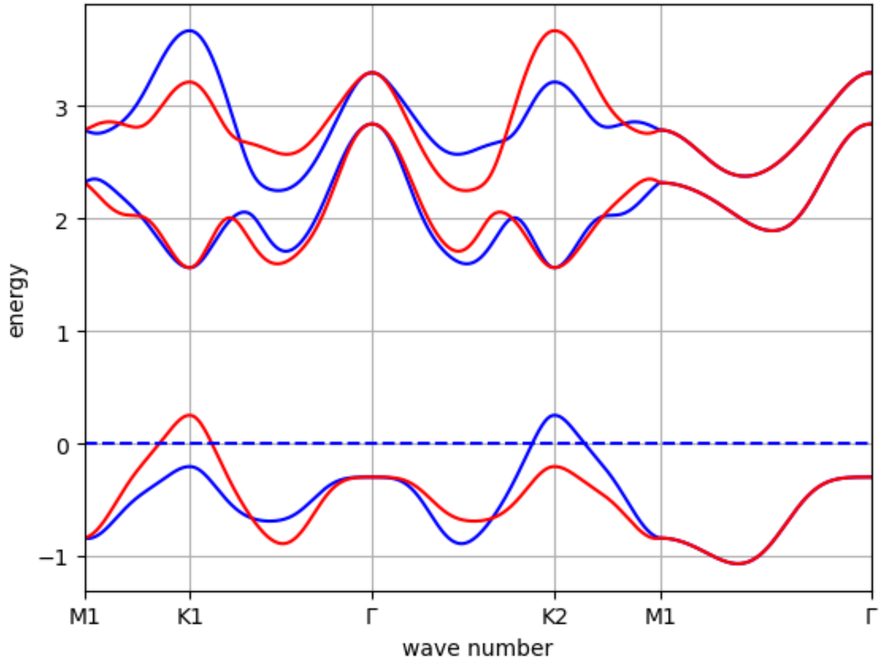
2.Habara, R. & Wakabayashi, K. Optically induced spin current in monolayer NbSe2. *Phys. Rev. B* **103**, L161410 (2021).

3.Zhou, B. T., Taguchi, K., Kawaguchi, Y., Tanaka, Y. & Law, K. T. Spin-orbit coupling induced valley Hall effects in transition-metal dichalcogenides. *Commun. Phys.* **2**, 26 (2019).

Compare WSe2 and WSeTe band structure

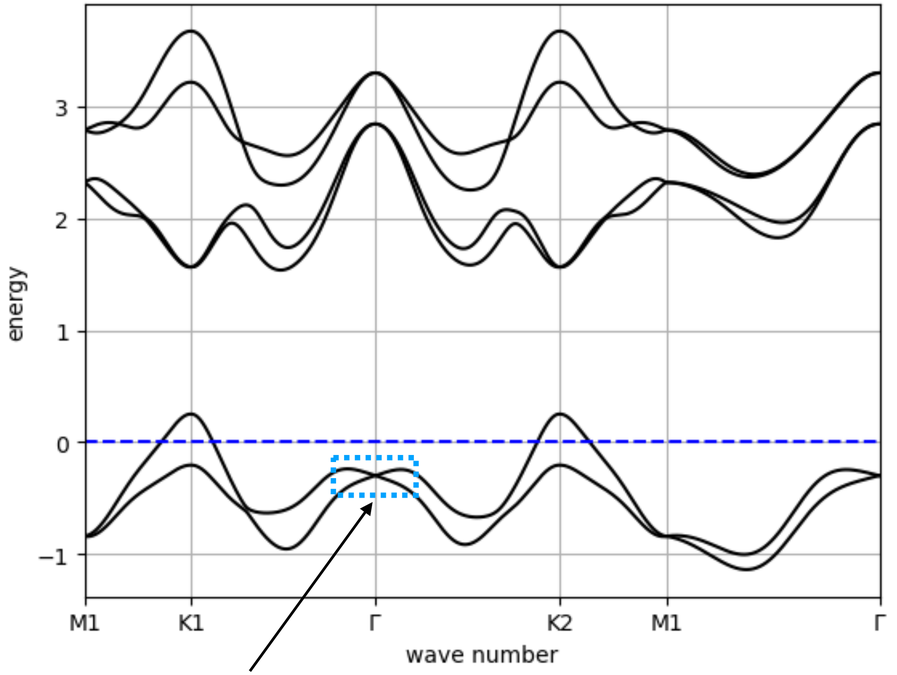
WSe2

$$H_{\mathrm{TB}}(\boldsymbol{k}) = \textcircled{1}\boxed{H_{\mathrm{TNN}}(\boldsymbol{k})\otimes\sigma_0} + \textcircled{2}\boxed{\frac{1}{2}\lambda L_z\otimes\sigma_z} + \textcircled{3}\boxed{} + \textcircled{4}\boxed{}$$



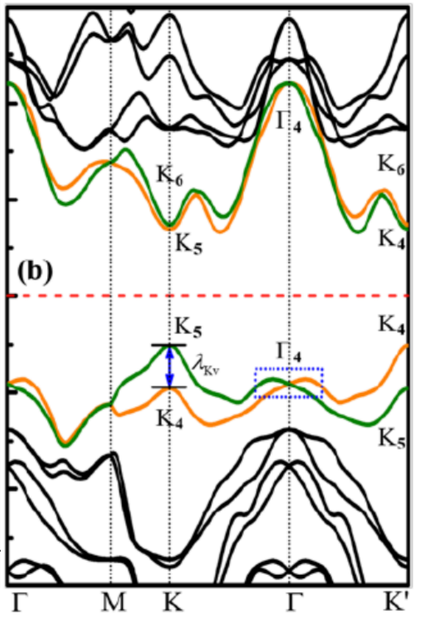
WSeTe

$$H_{\mathrm{TB}}(\boldsymbol{k}) = \textcircled{1}\boxed{H_{\mathrm{TNN}}(\boldsymbol{k})\otimes\sigma_0} + \textcircled{2}\boxed{\frac{1}{2}\lambda L_z\otimes\sigma_z} + \textcircled{3}\boxed{H_{\mathrm{R}}(\boldsymbol{k})} + \textcircled{4}\boxed{}$$



Rashba効果によるスピン分裂

DFT calculation



先行研究結果

Yao, Qun-Fang & Cai, Jia & Tong, Wen-Yi & Gong, Shi-Jing & Wang, Ji-Qing & Wan, Xian-gang & Duan, Chun-Gang & Chu, J.. (2016).

Parameters were taken from the following paper

1.Liu, G., Shan, W., Yao, Y., Yao, W. & Xiao, D. Three-band tight-binding model for monolayers of group-VIB transition metal dichalcogenides. *Phys. Rev. B* **88**, 085433 (2013).

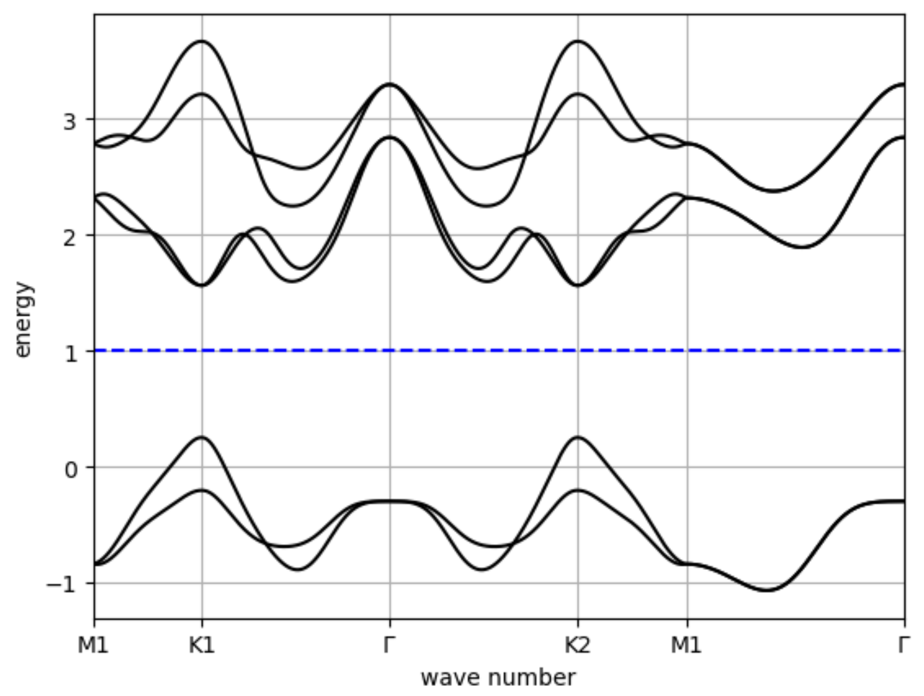
2.Zhou, B. T., Taguchi, K., Kawaguchi, Y., Tanaka, Y. & Law, K. T. Spin-orbit coupling induced valley Hall effects in transition-metal dichalcogenides. *Commun. Phys.* **2**, 26 (2019).

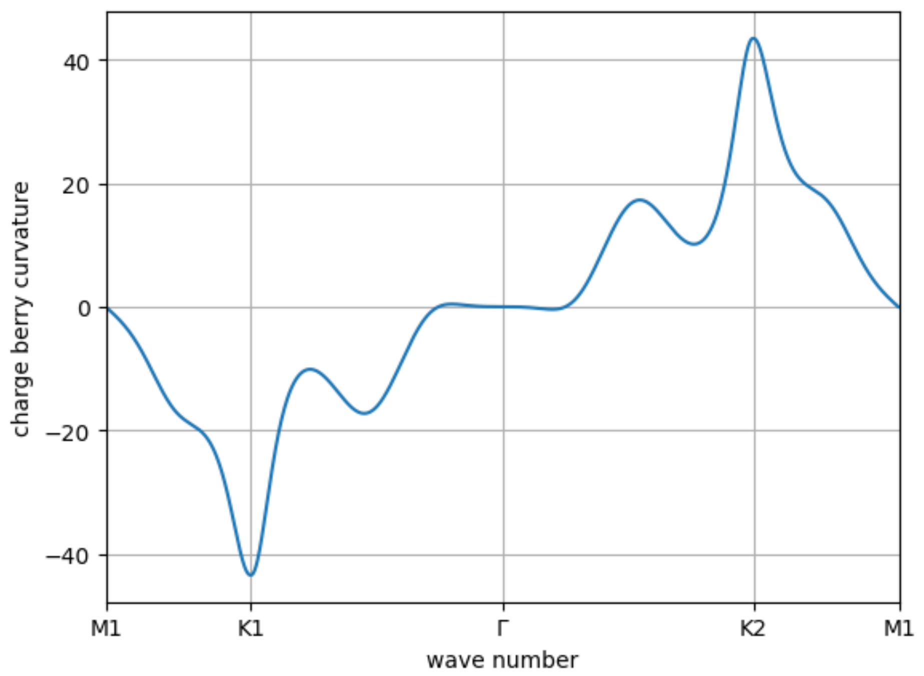
Compare WSe2 and WSeTe

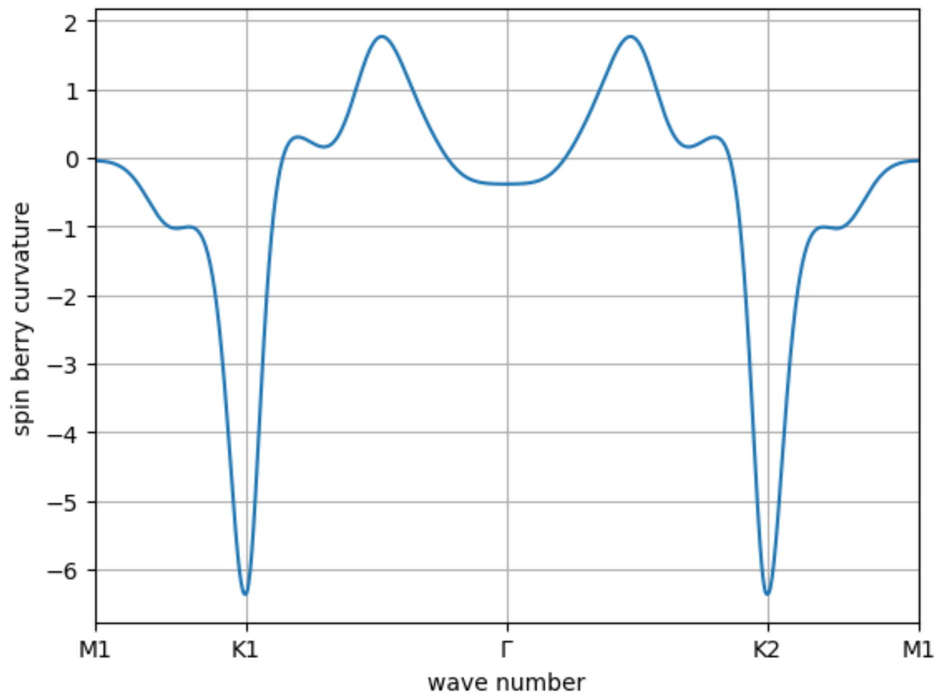
WSe2

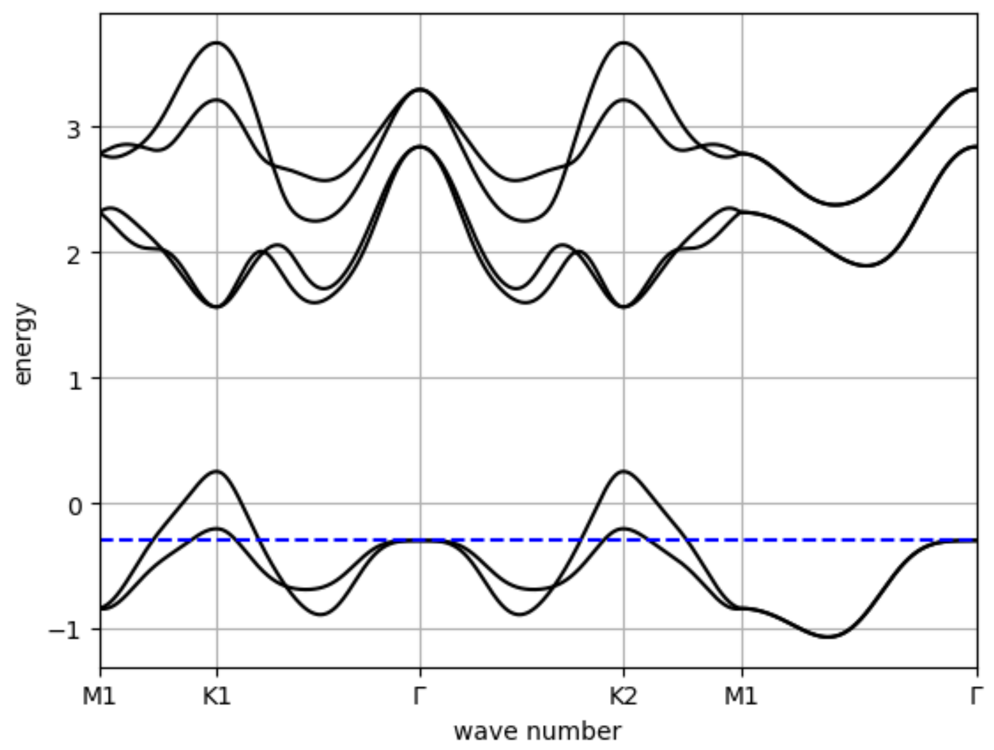
Charge BC

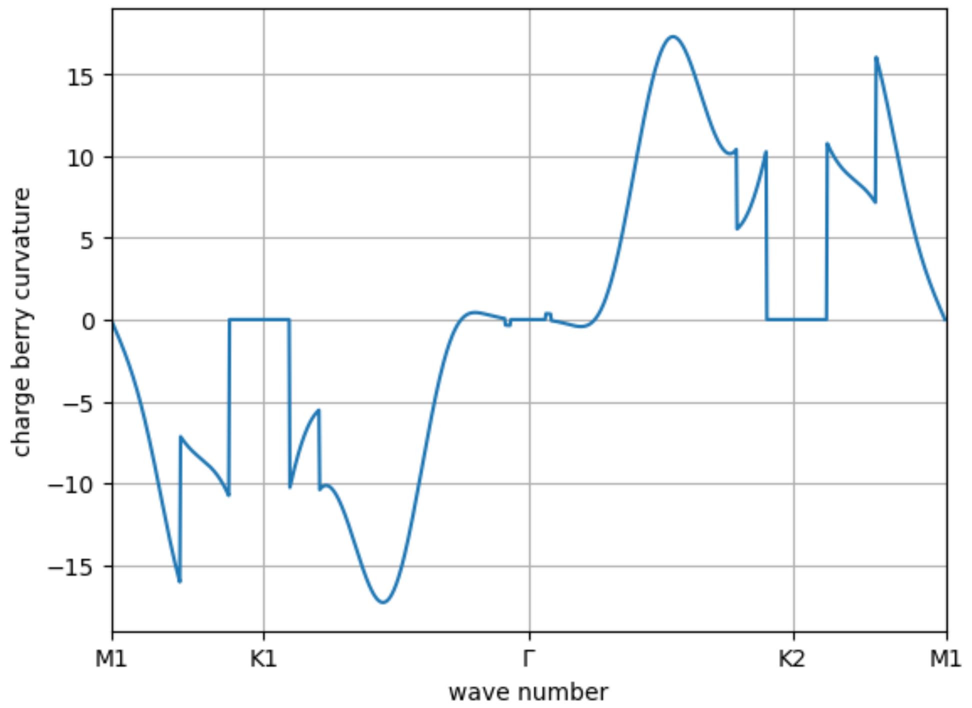
Spin BC

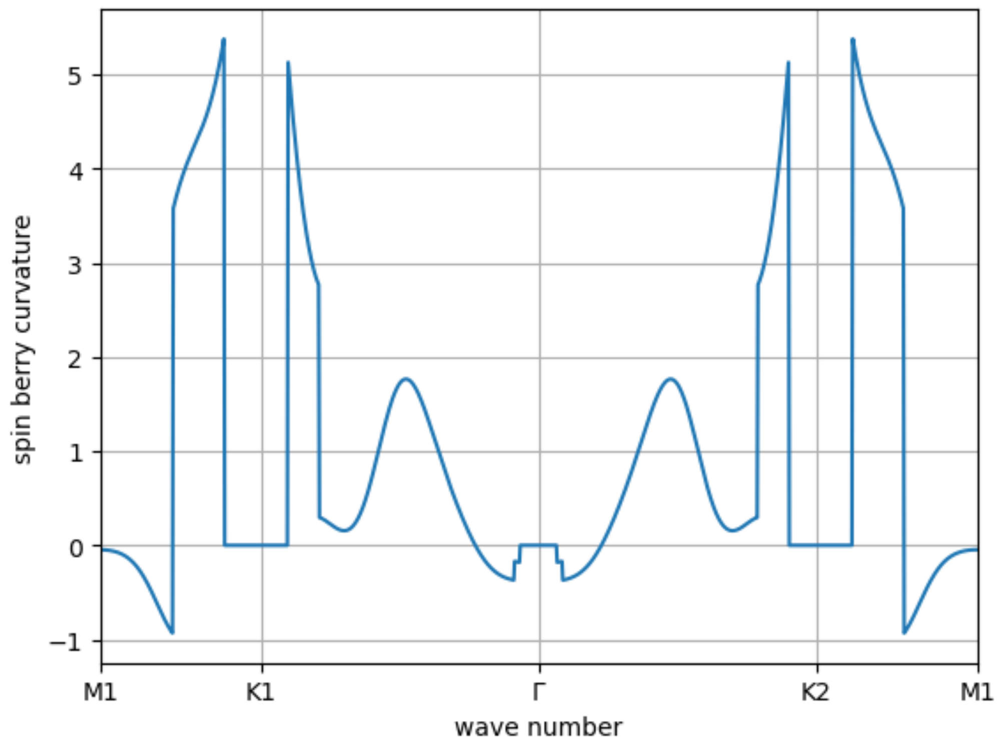


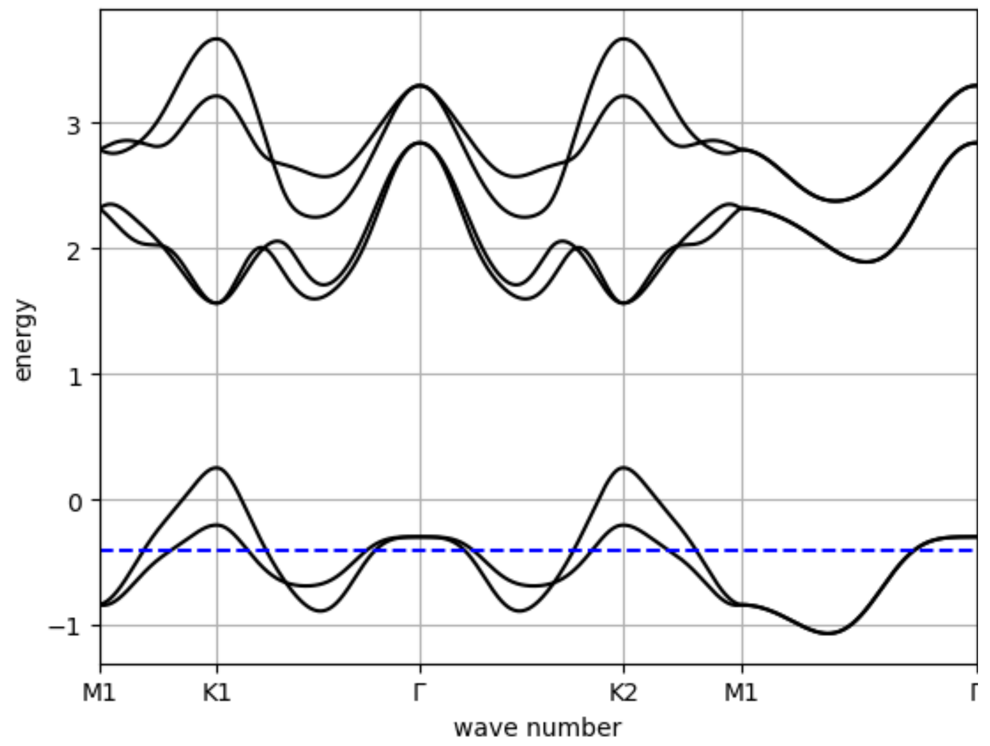


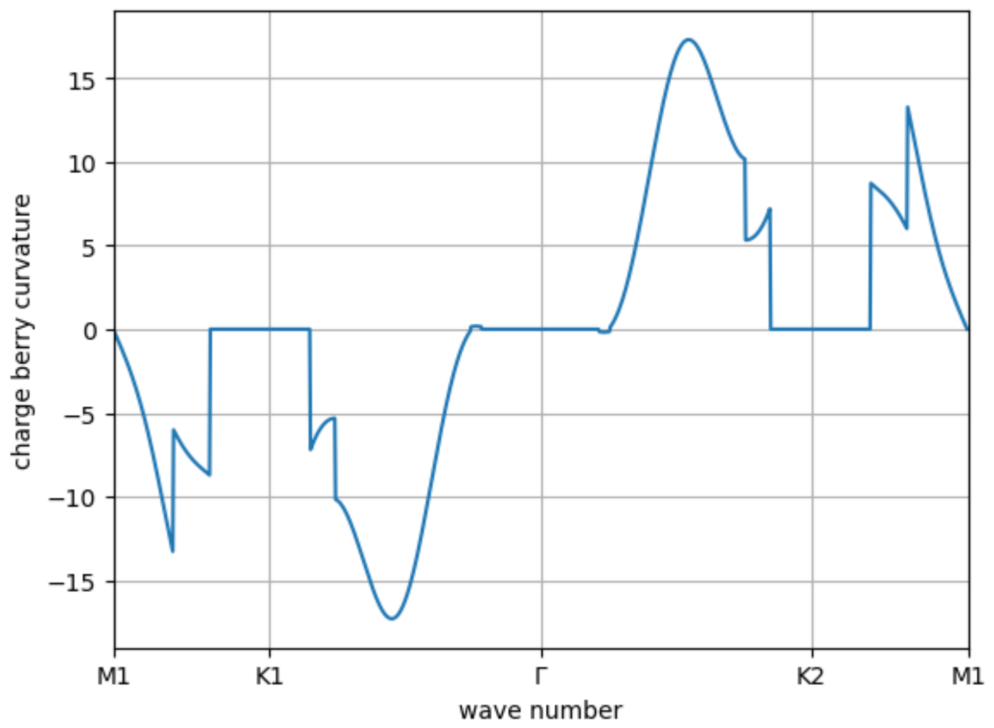


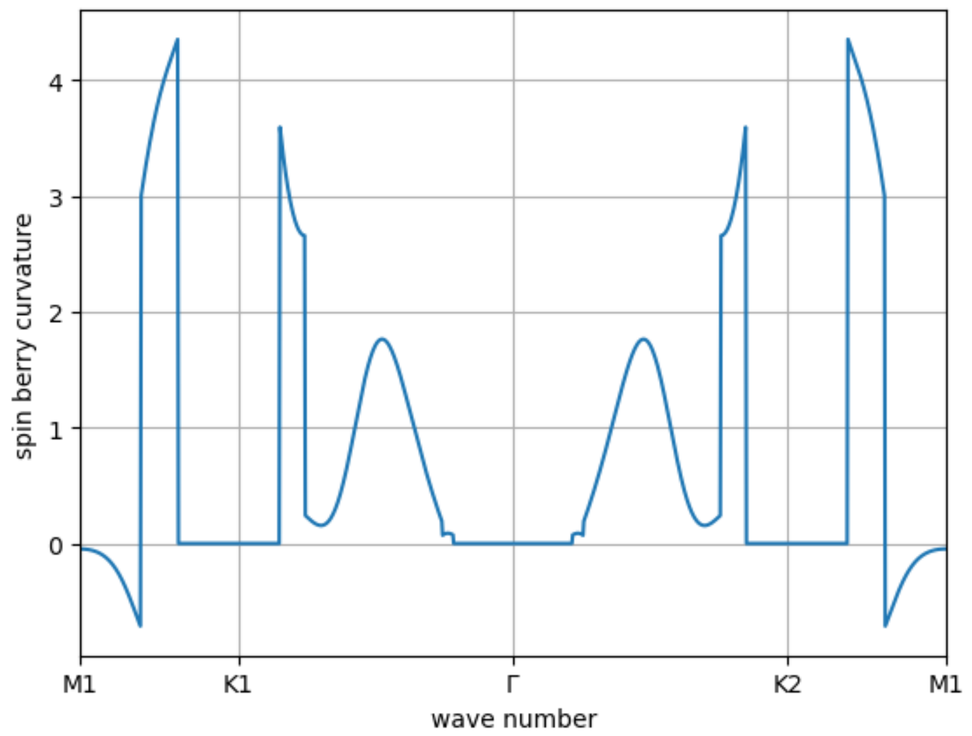












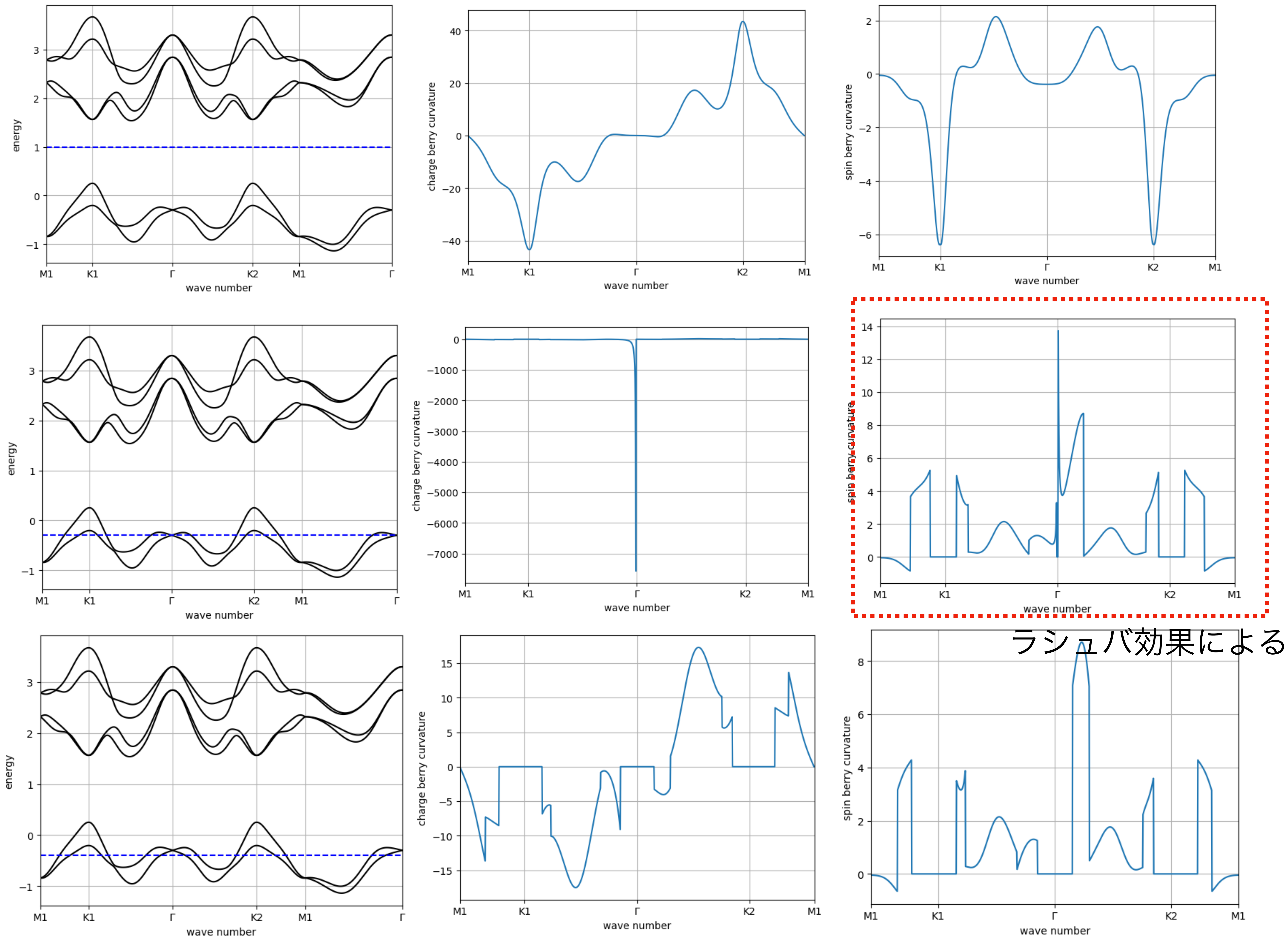
Compare WSe2 and WSeTe

$$\Omega^{s_z}_{n,xy}(\boldsymbol{k}) = \hbar\sum_{m\neq n}\frac{-2\mathrm{Im}\left[\langle n\boldsymbol{k}|\hat{j}^z_x|m\boldsymbol{k}\rangle\langle m\boldsymbol{k}|\hat{v}_y|n\boldsymbol{k}\rangle\right]}{(E_{n\boldsymbol{k}}-E_{m\boldsymbol{k}})^2}$$

WSeTe

Charge BC

Spin BC

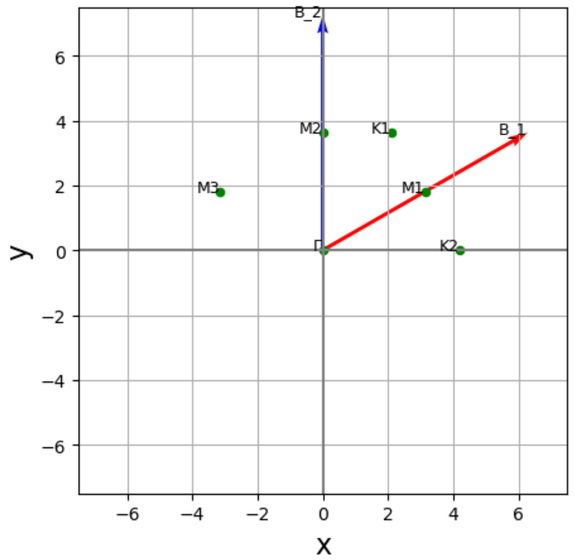


ラシュバ効果によるスピン分裂->Spin BCが大きくなる

Next

- Rashba parameter
- Wannier 90 -> BC計算
- Other Janus TMDC
- Spin hall conductivity

$$\Omega_{n,xy}^{s_z}(\boldsymbol{k}) = \hbar \sum_{m \neq n} \frac{-2\mathrm{Im}\left[\langle n\boldsymbol{k}|\hat{j}_x^z|m\boldsymbol{k}\rangle\langle m\boldsymbol{k}|\hat{v}_y|n\boldsymbol{k}\rangle\right]}{(E_{nk} - E_{mk})^2}$$



- Three band tight binding model with Ising type SOC and Rashba type SOC
- Plot charge berry curvature and spin berry curvature
- Compared WSe2 and WSeTe about electrical properties