Symmetry and Geometric Phases

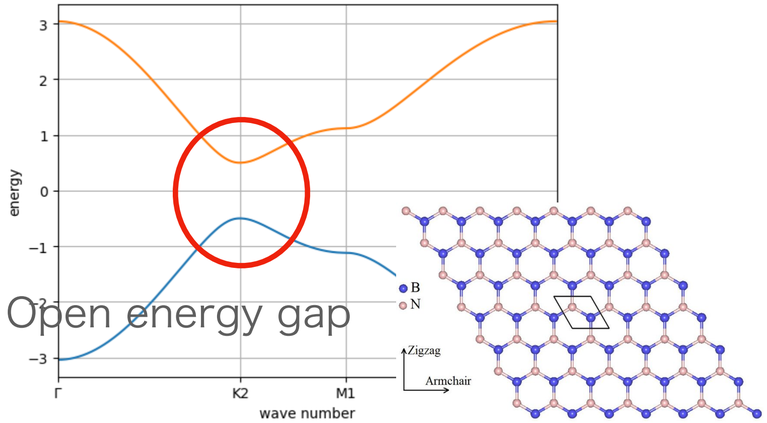
Introduction to Berry Phase

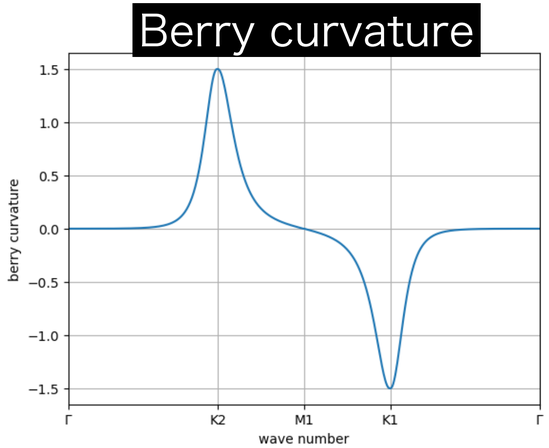
Tomoaki Kameda 12 June 2024

Review of previous seminar

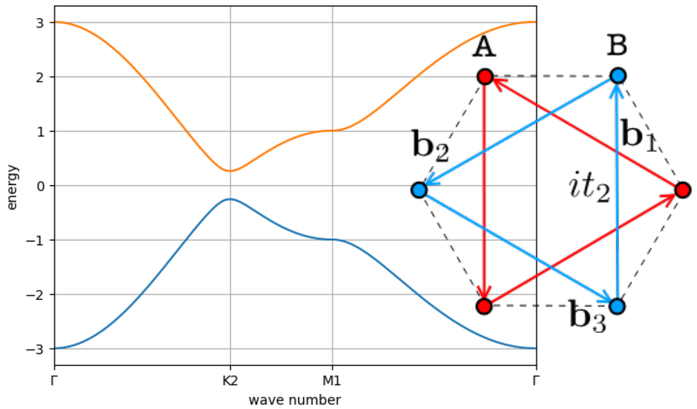
Breaking symmetry

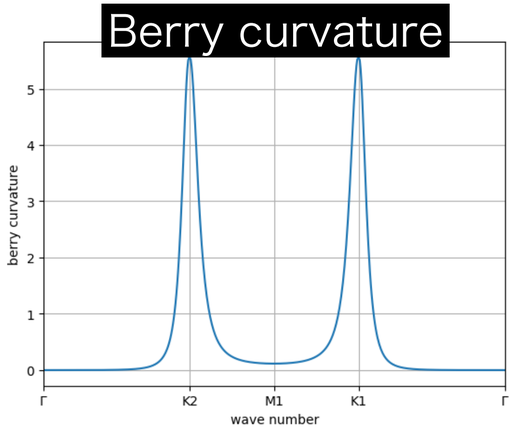
BC is odd-function in h-BN model (breaking inversion symmetry)





BC is even-function in Haldane model (breaking time reversal symmetry)





Todays seminar topics

Symmetry and geometric phases

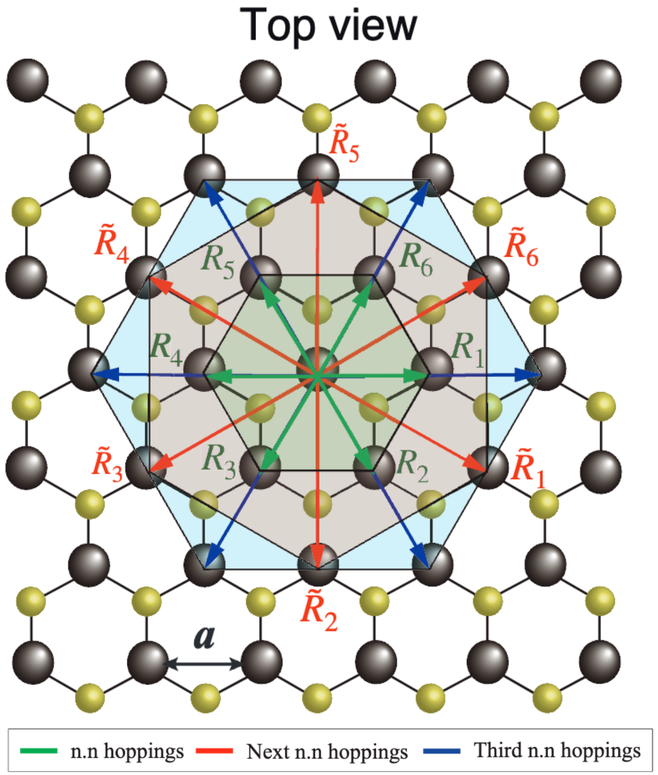
- Why Berry curvature is changed with broken symmetry?
- consider the symmetry in quantum mechanics in order to understand above it.

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).

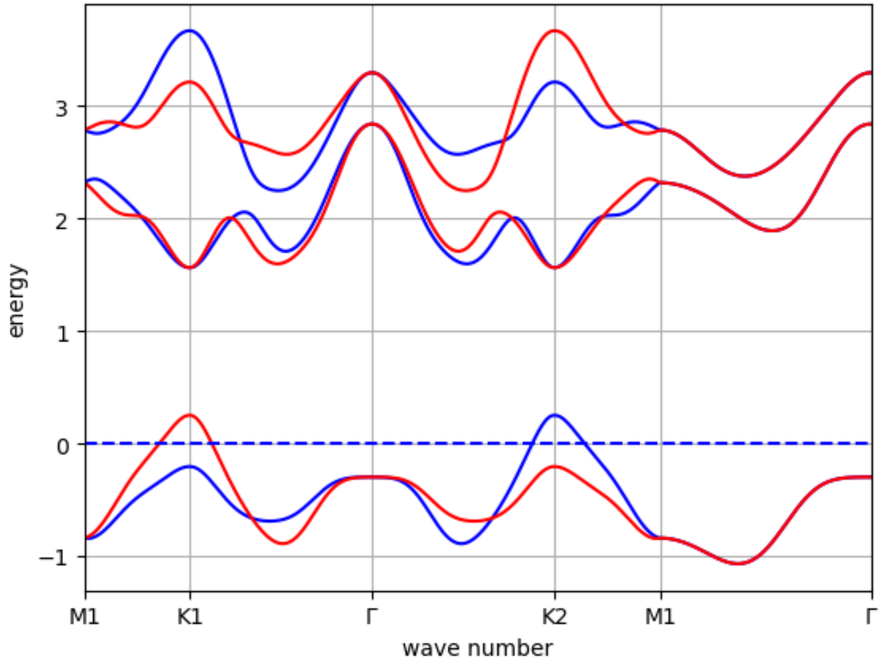
2.Habara, R. & Wakabayashi, K. Optically induced spin current in monolayer NbSe2. *Phys. Rev. B* **103**, L161410 (2021).

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

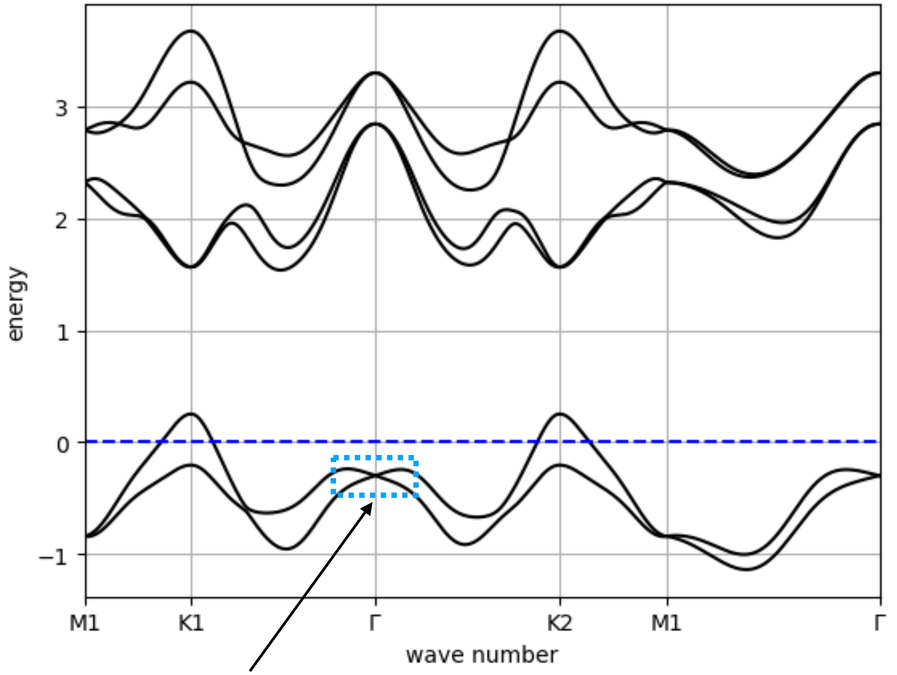
WSe2

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



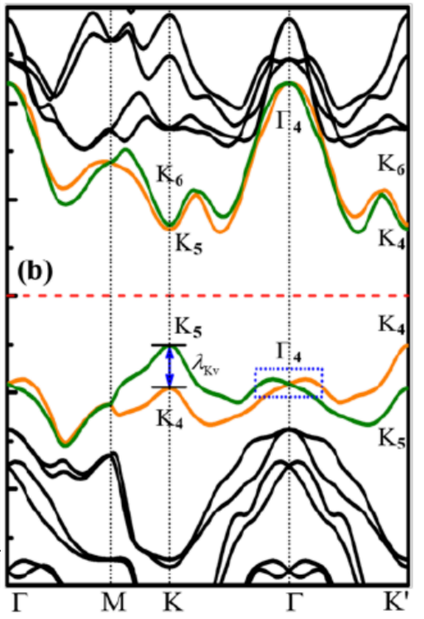
WSeTe

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



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).

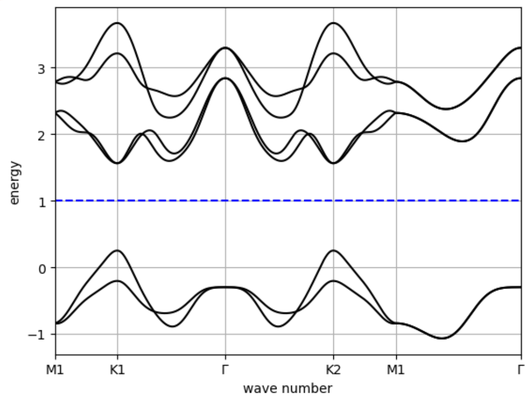
Compare WSe2 and WSeTe

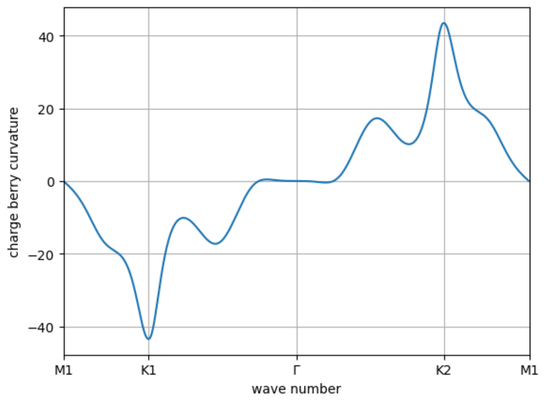
WSe2

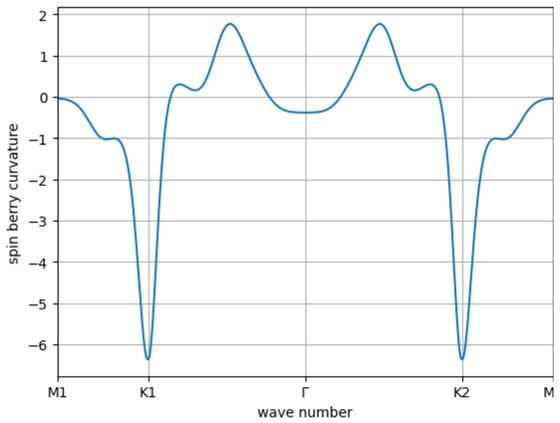
Charge BC

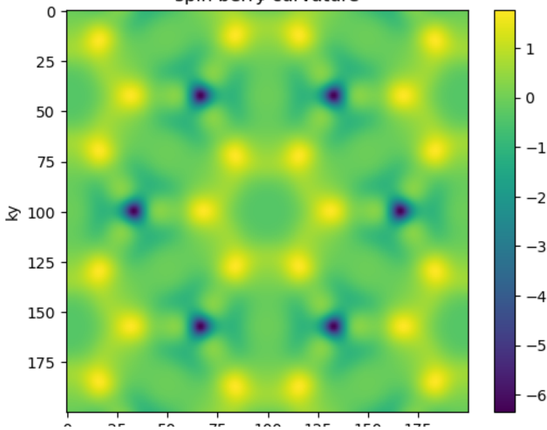
Spin BC

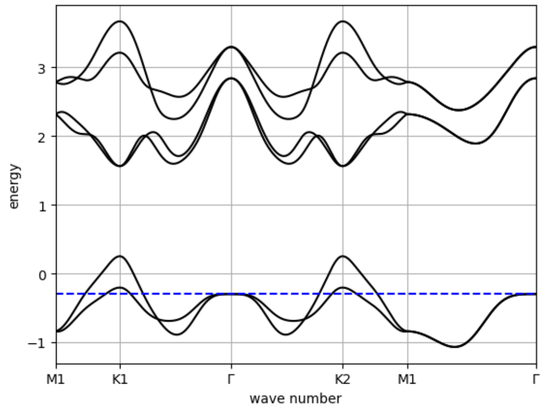
Spin BC

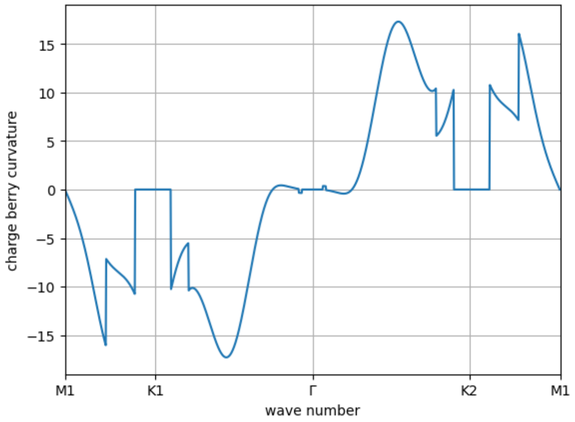


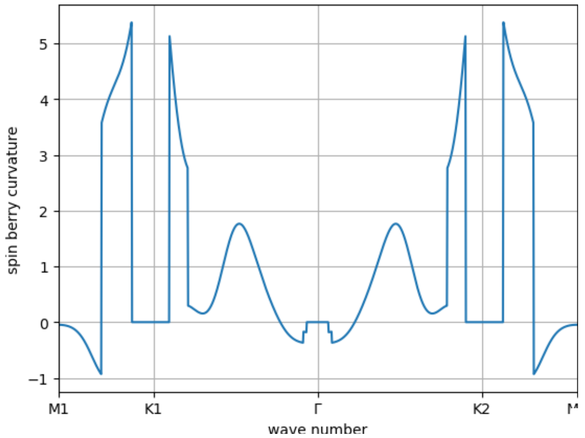


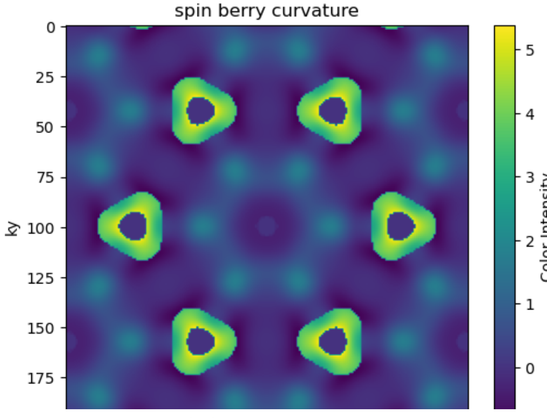


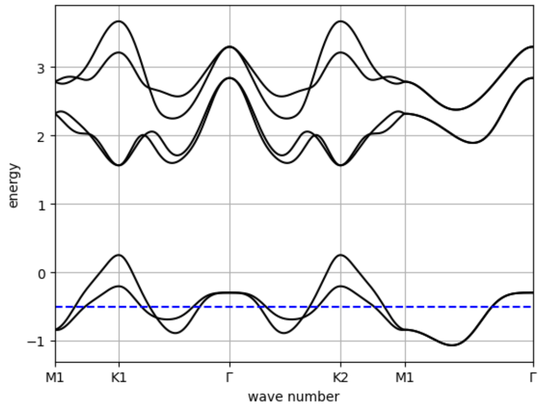


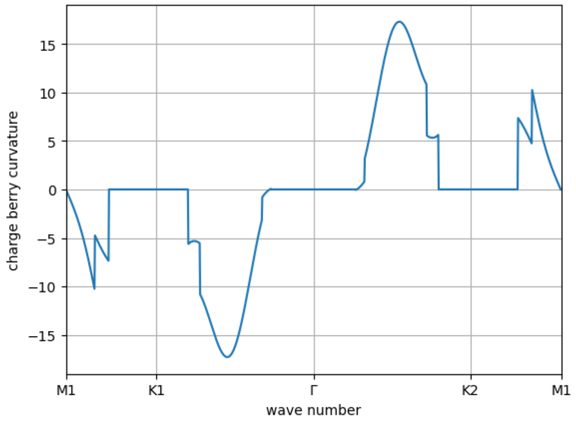


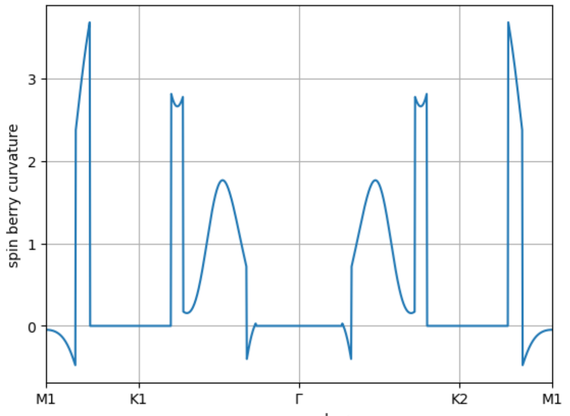


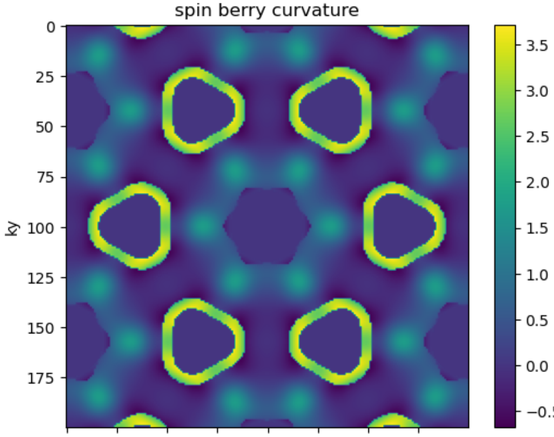












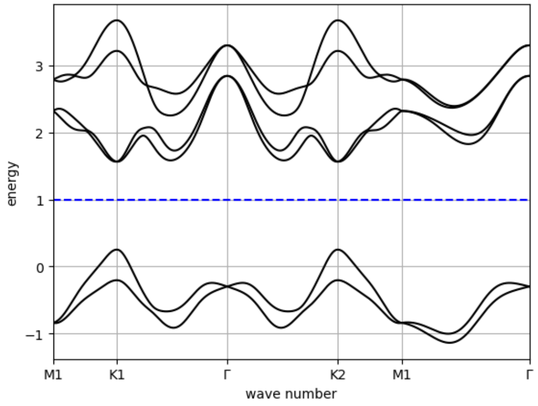
Compare WSe2 and WSeTe

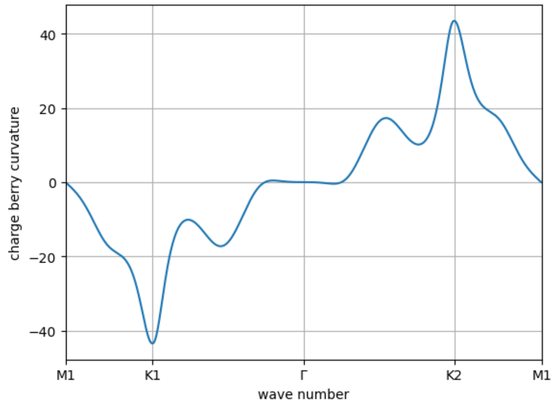
$$\Omega_{n,xy}^{s_z}(\boldsymbol{k}) = \hbar \sum_{m \neq n} \frac{-2\mathrm{Im}\left[\langle n\boldsymbol{k}|\hat{j}_x^z|m\boldsymbol{k}\rangle \langle m\boldsymbol{k}|\hat{v}_y|n\boldsymbol{k}\rangle\right]}{(E_{nk} - E_{mk})^2}$$

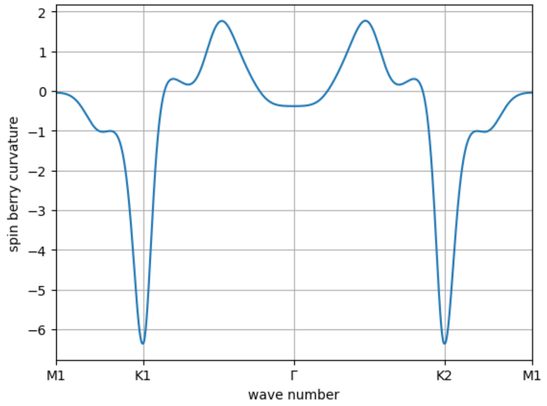
WSeTe

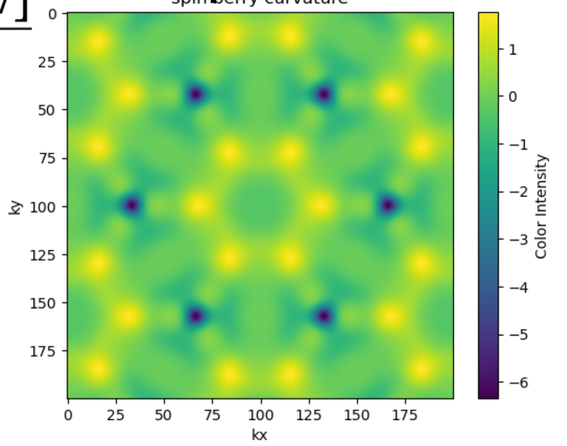
Charge BC

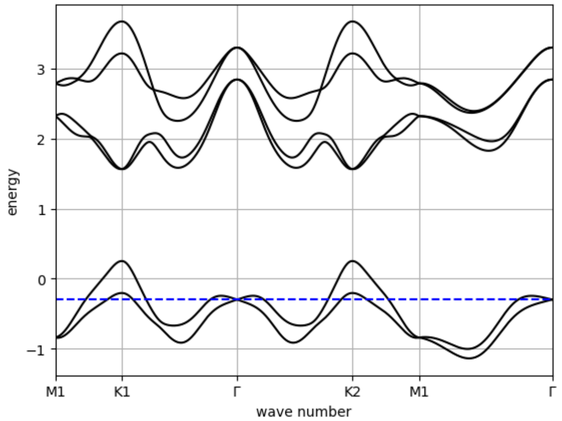
Spin BC

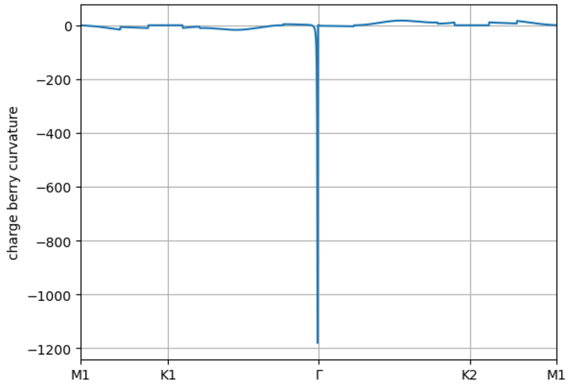


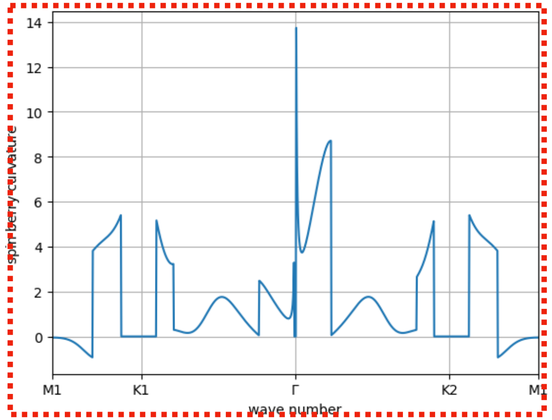


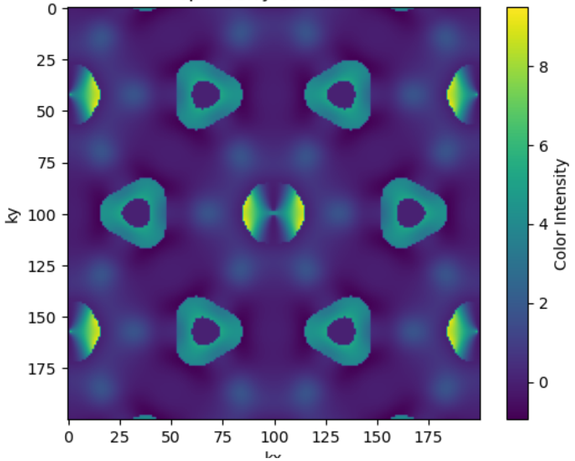


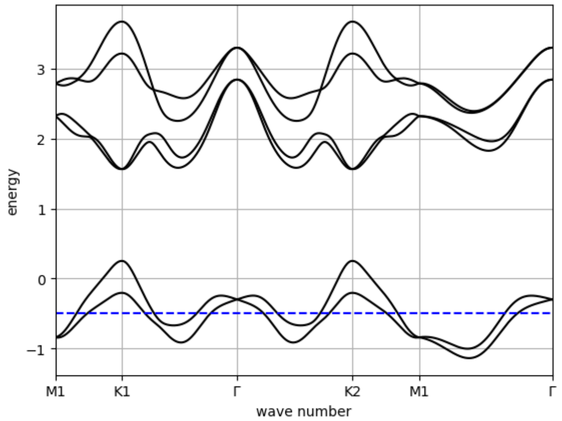


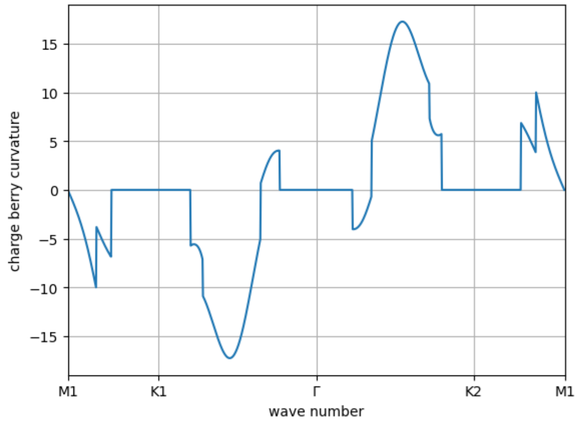


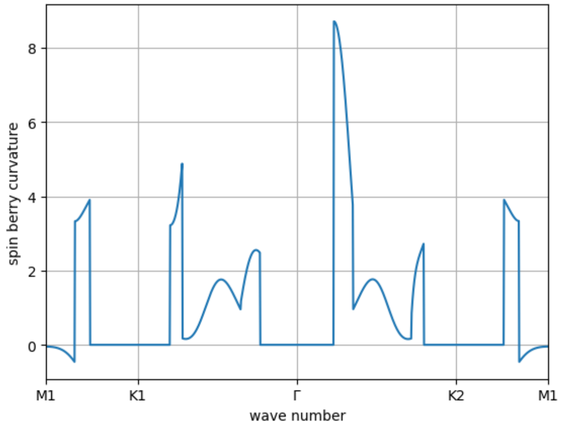


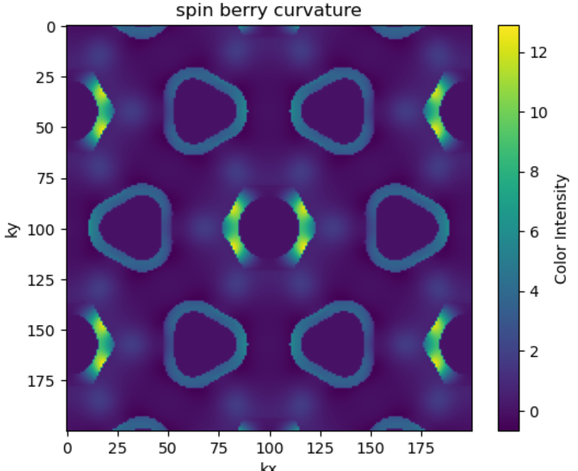












Berry curvature of $NbSe_2$

previous studies

PHYSICAL REVIEW B **103**, L161410 (2021)

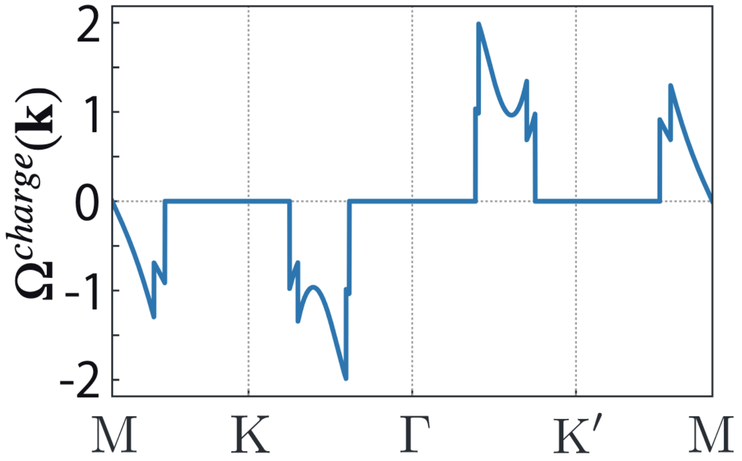
Optically induced spin current in monolayer $NbSe_2$

Ren Habara [1] and Katsunori Wakabayashi [1,2,3]

Objective:

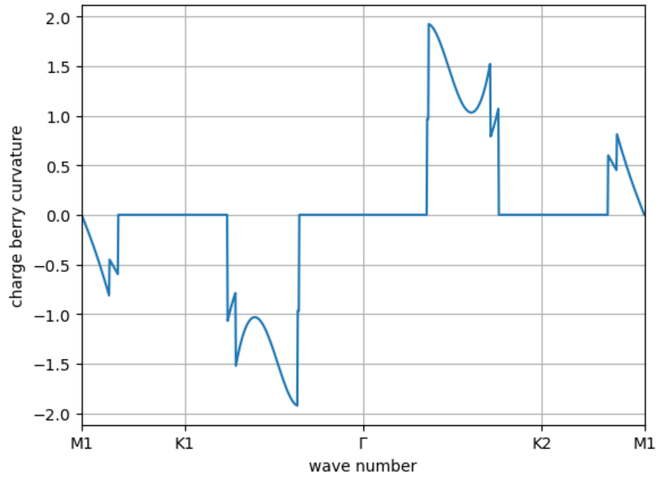
・ensure that **Charge** and **Spin Berry curvature** are correct by comparing with previous studies.

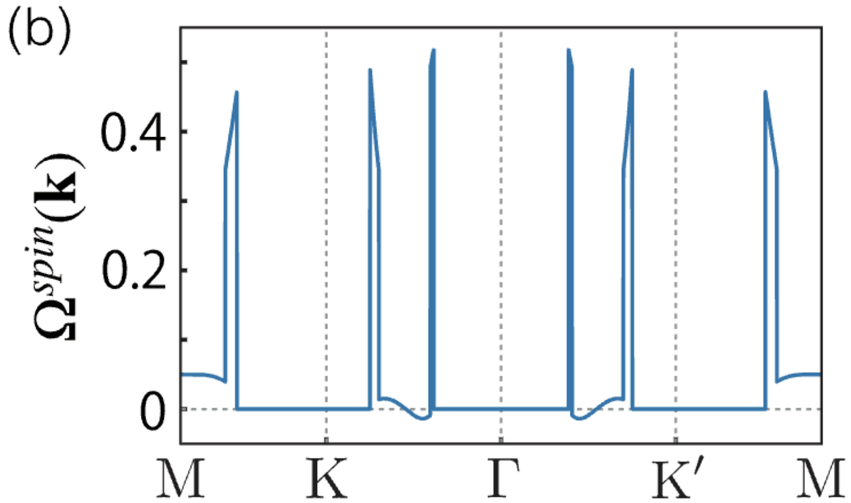
Results of previous studies



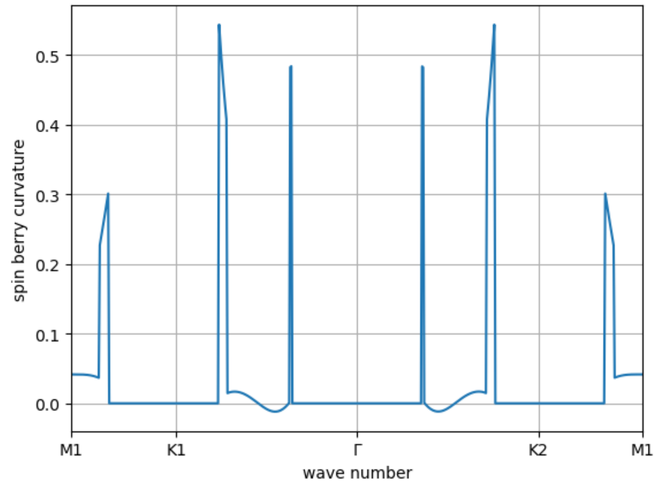
Charge BC

My calculation





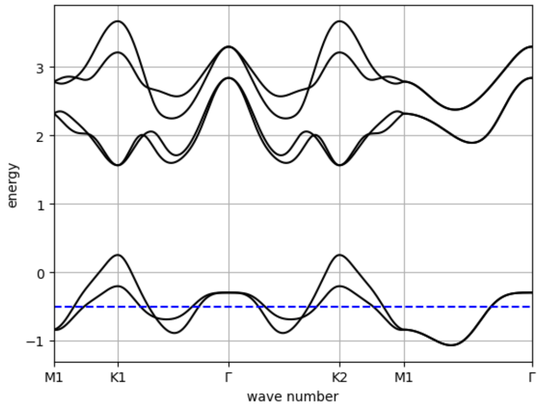
Spin BC

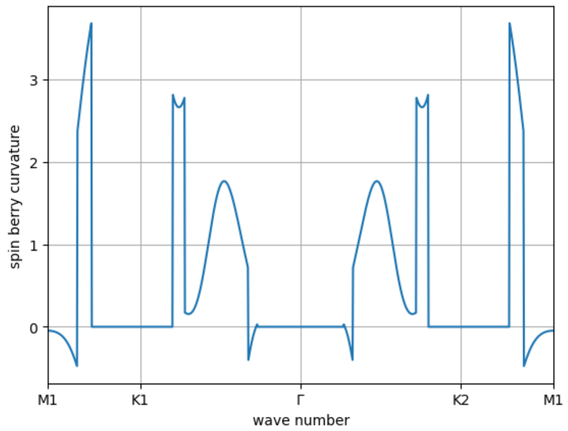


DC limit conductivity (spin hall conductivity)

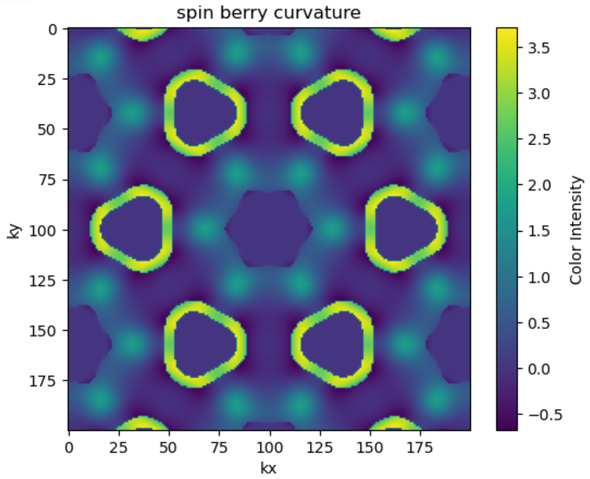
Not yet

WSe2

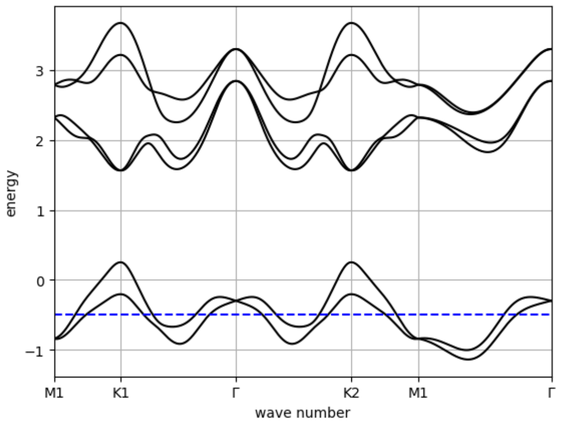


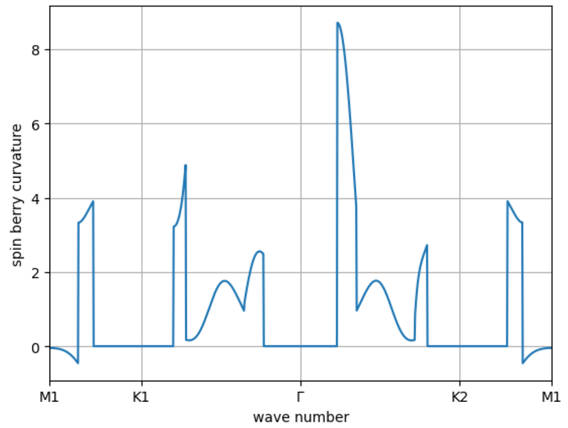


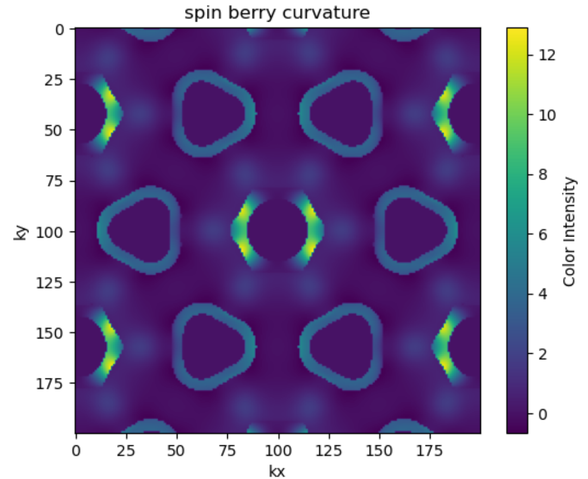
Spin BC



WSeTe







Optical Conductivity of $NbSe_2$

previous studies

PHYSICAL REVIEW B **103**, L161410 (2021)

Optically induced spin current in monolayer $NbSe_2$

Ren Habara[1] and Katsunori Wakabayashi[1,2,3]

Objective:

・ensure that optical conductivity calculation is correct by comparing with previous studies.

Berry curvature considering spin orbit coupling

$$\Omega^{charge}(\boldsymbol{k}) = \Omega^{\uparrow}(\boldsymbol{k}) + \Omega^{\downarrow}(\boldsymbol{k})$$

$$= \hbar^2 \sum_n f(E_{n\boldsymbol{k}}) \sum_{m \neq n} \frac{-2\mathrm{Im}\,\langle u_{n\boldsymbol{k}}|\hat{v}_x|u_{m\boldsymbol{k}}\rangle \langle u_{m\boldsymbol{k}}|\hat{v}_y|u_{n\boldsymbol{k}}\rangle}{(E_{m\boldsymbol{k}} - E_{n\boldsymbol{k}})^2}.$$

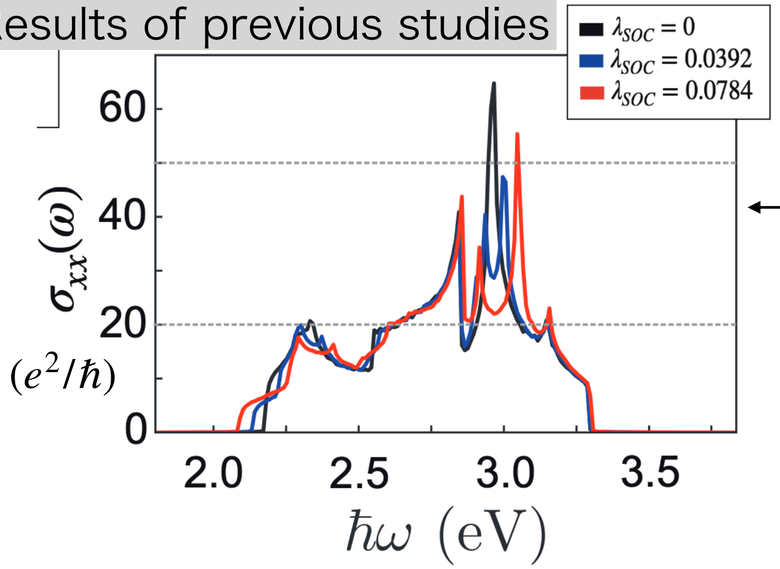
Optical longitudinal conductivity σxx(ω) of monolayer NbSe2

Problem

・WF is not collect ?

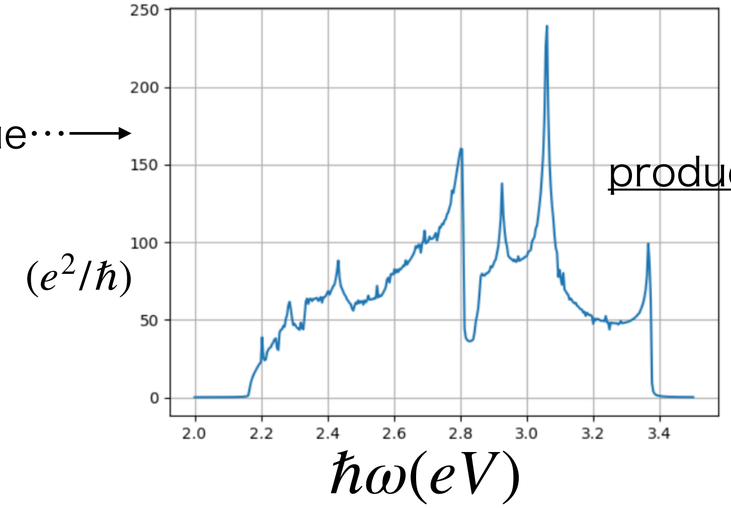
Degeneracy

Results of previous studies



←Difference value…→

My calculation $\lambda_{SOC} = 0.0784$



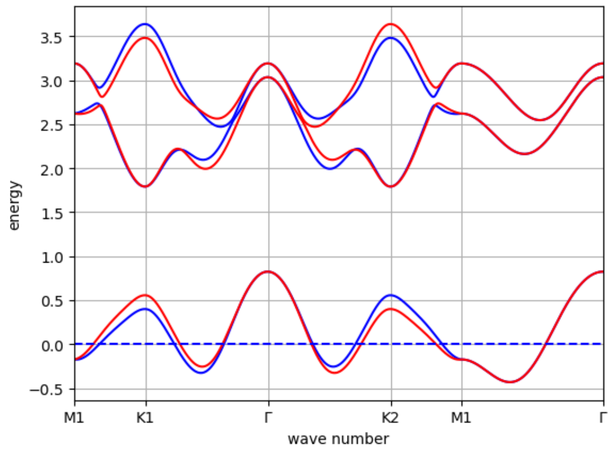
produce different calculation results.

Calculate conductivity up and down spin, respectively.

Calculate conductivity using total hamiltonian.

Energy band structure of $NbSe_2$

Calculate up and down spin (spin z component) hamiltonian, respectively

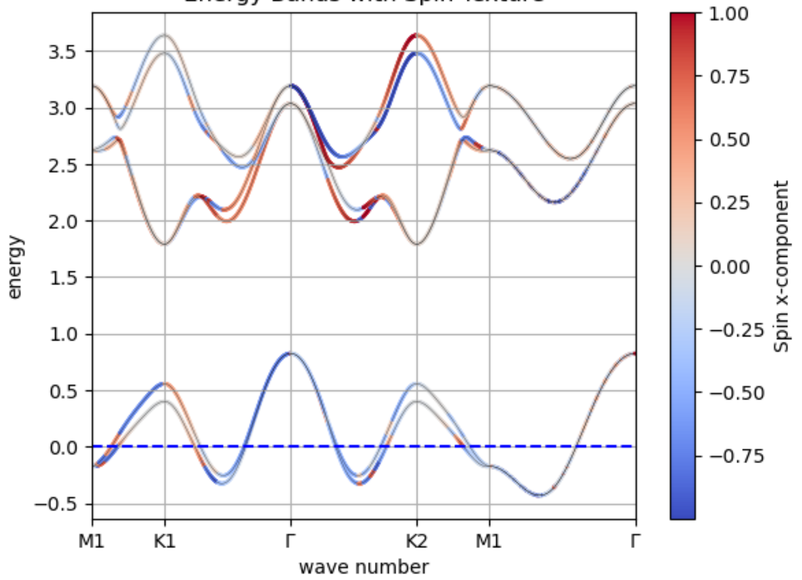


Hamiltonian

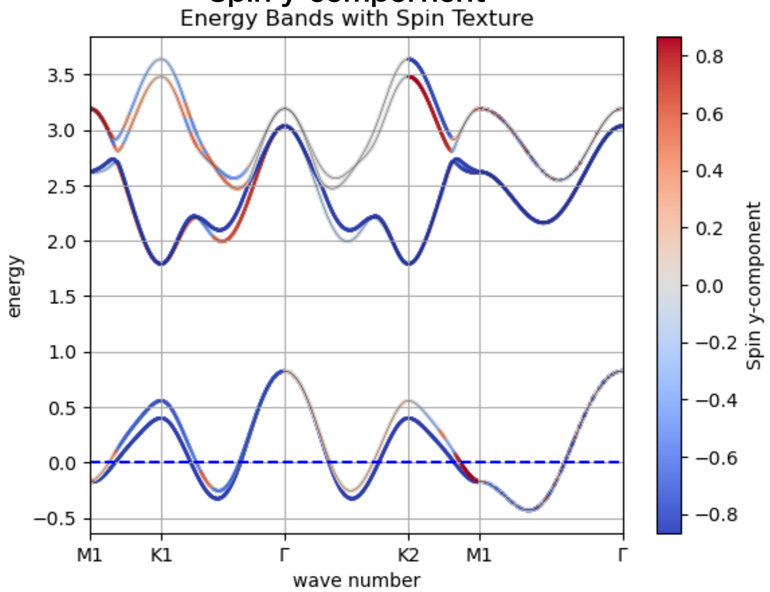
Problem
・WF is not collect ?
Degeneracy

Calculate total hamiltonian(and plot with spin component)

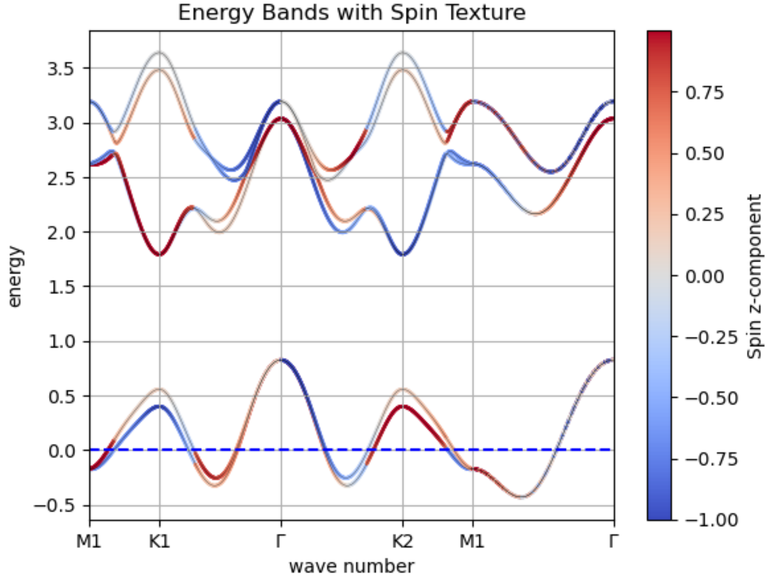
Spin x-compornent



Spin y-compornent

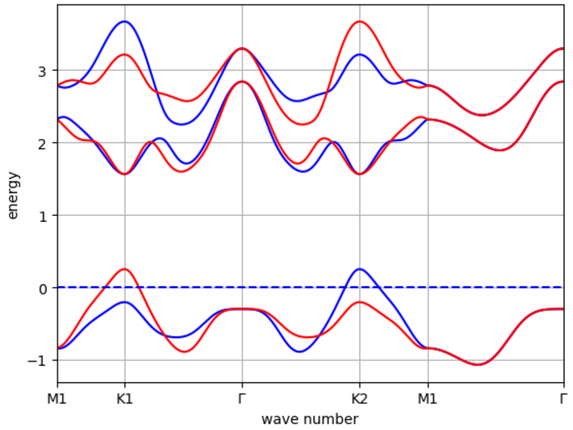


Spin z-compornent



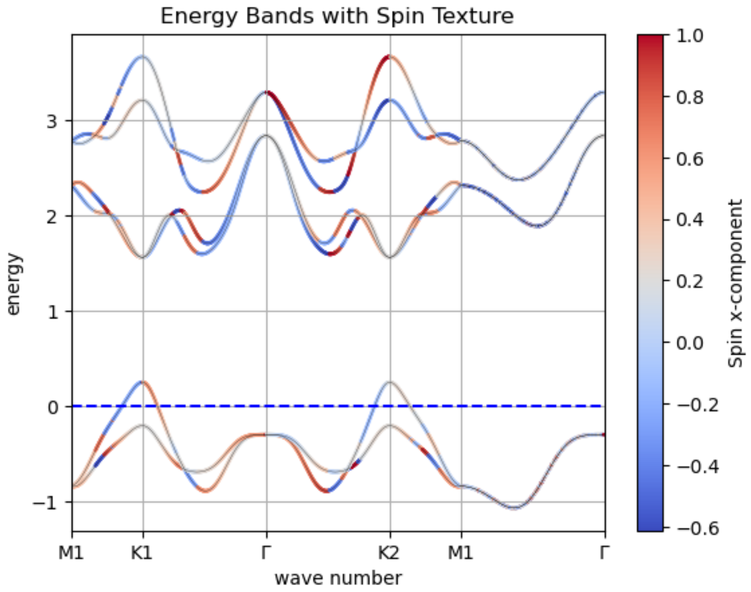
Energy band structure of WSe_2

Calculate up and down spin (spin z component) hamiltonian, respectively

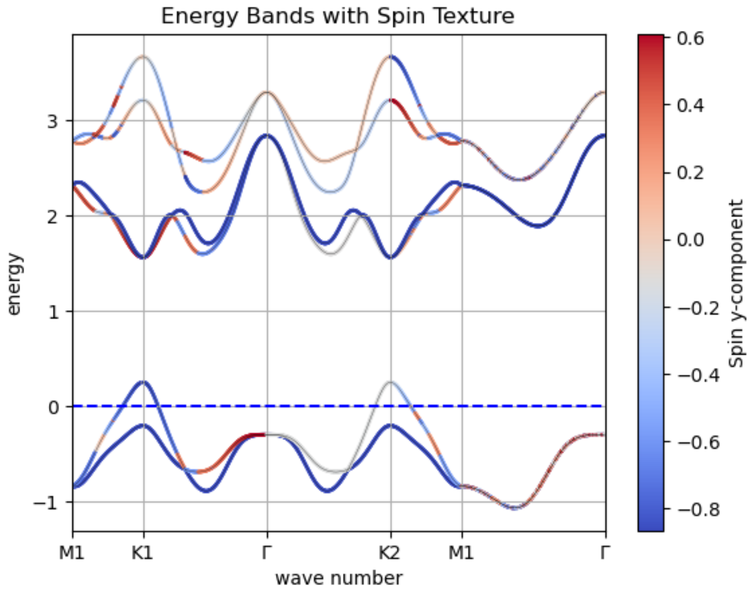


Calculate total hamiltonian(and plot with spin component)

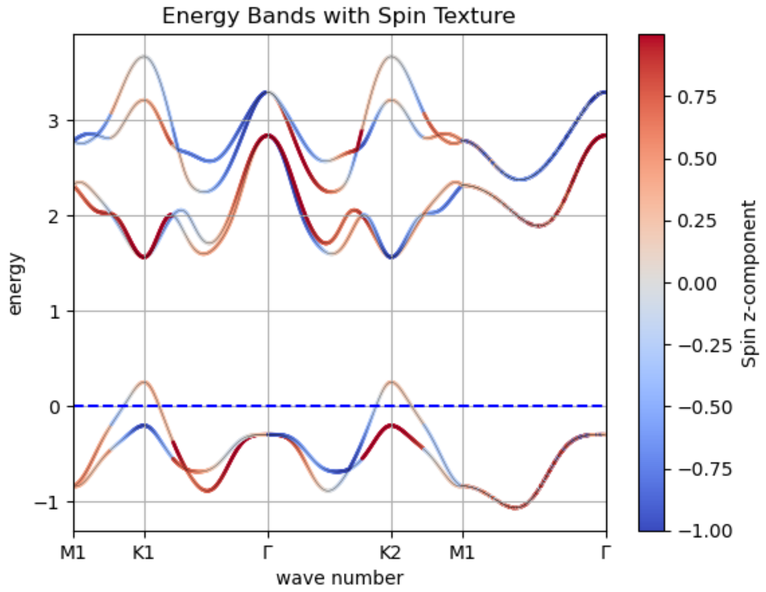
Spin x-compornent



Spin y-compornent

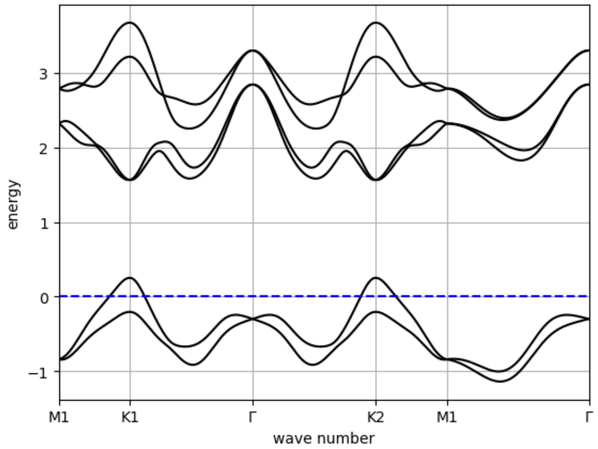


Spin z-compornent

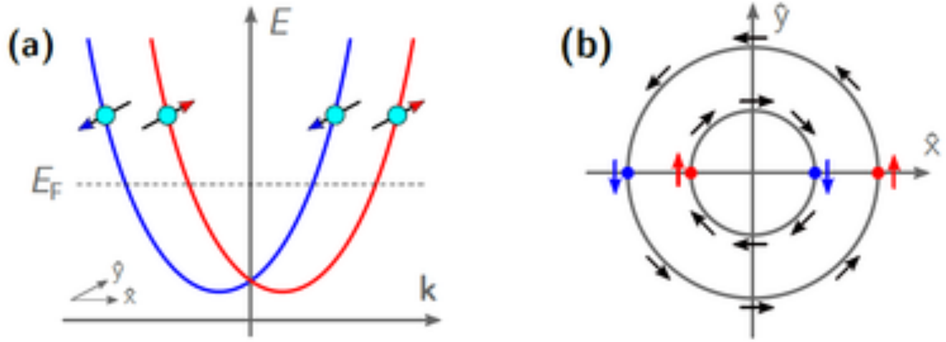


Energy band structure of WSeTe

Calculate total hamiltonian without spin component

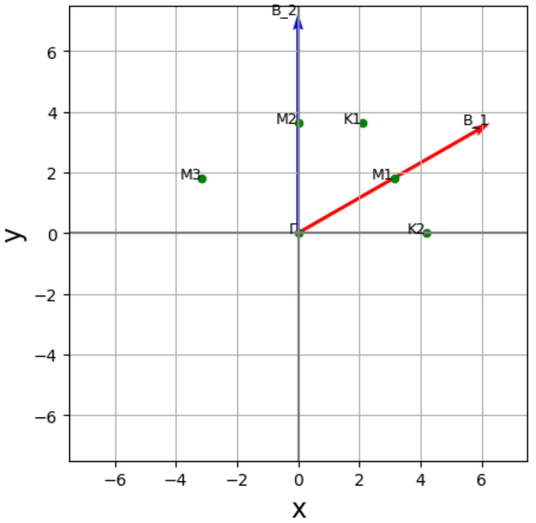


Rashba effect spin splitting



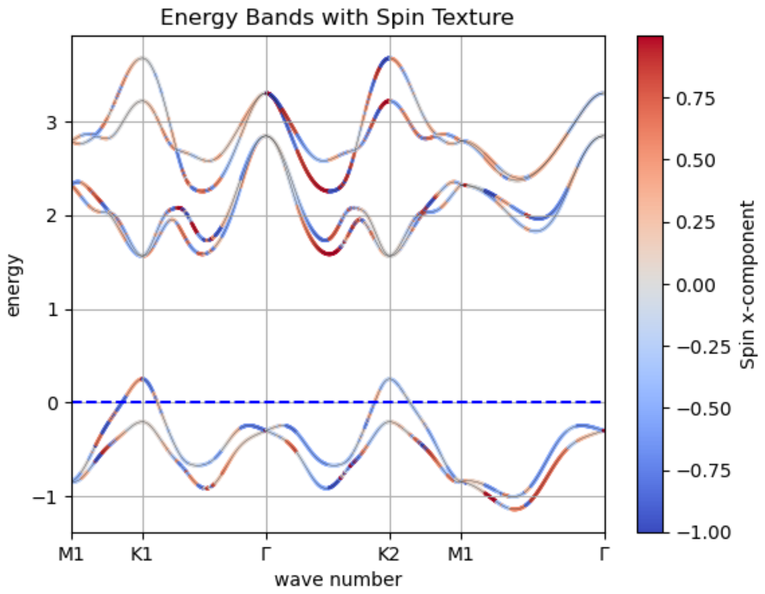
https://en.wikipedia.org/wiki/Rashba%E2%80%93Edelstein_effect

ブリユアンゾーン

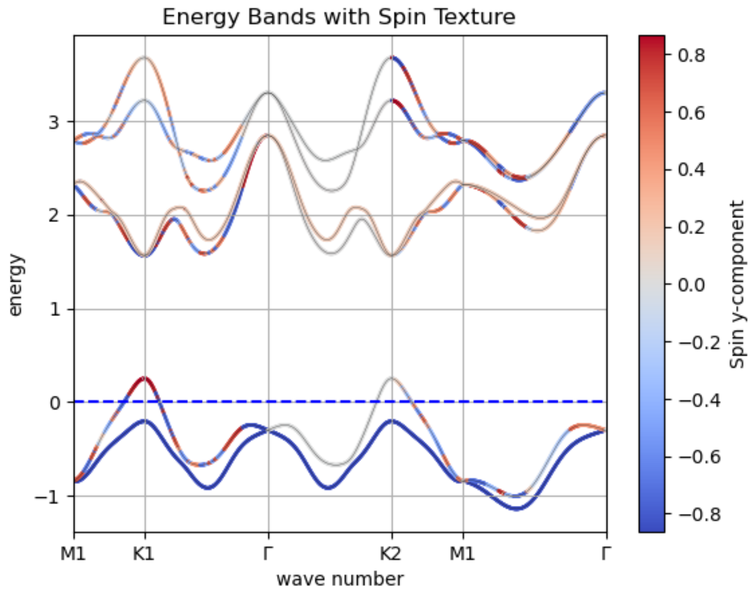


Calculate total hamiltonian(and plot with spin component)

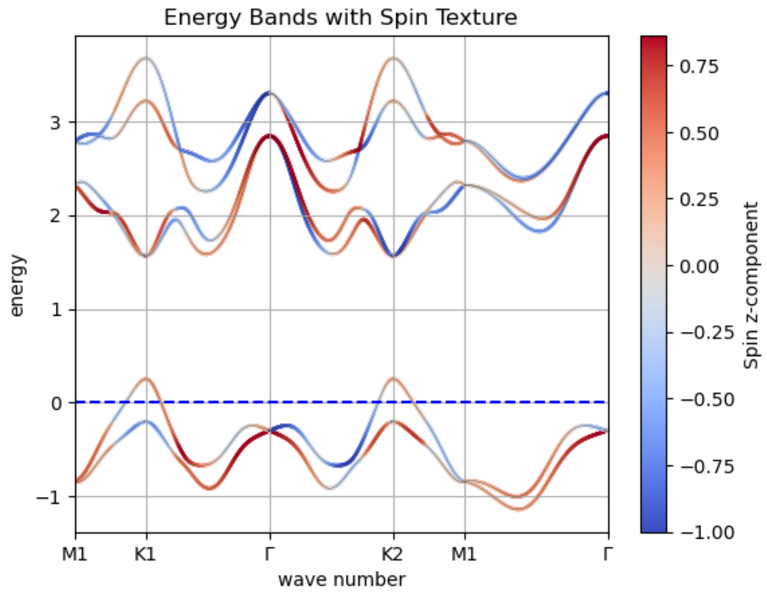
Spin x-compornent



Spin y-compornent

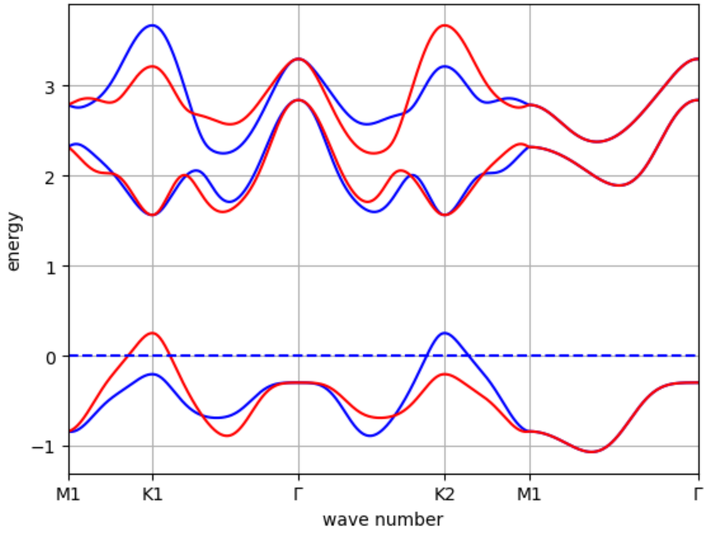


Spin z-compornent

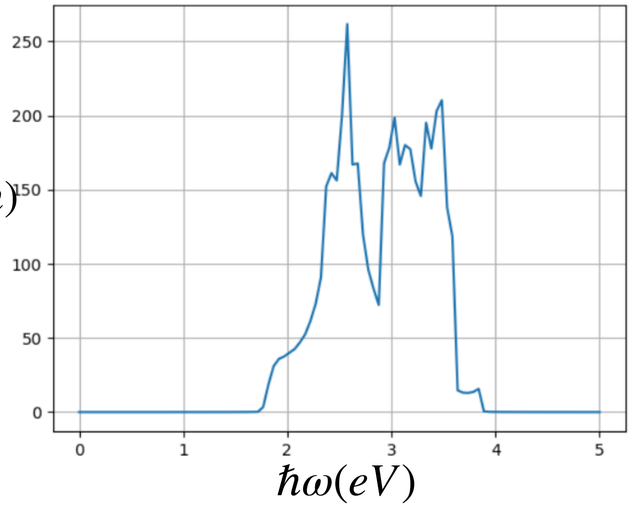


Optical conductivity of WSe_2

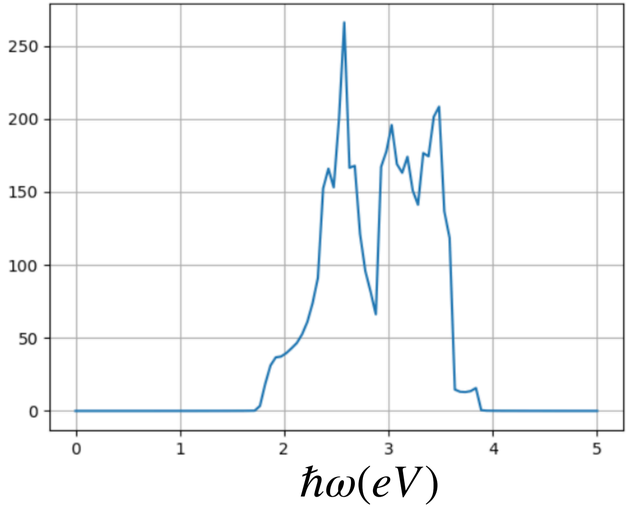
Chemical potential = 0



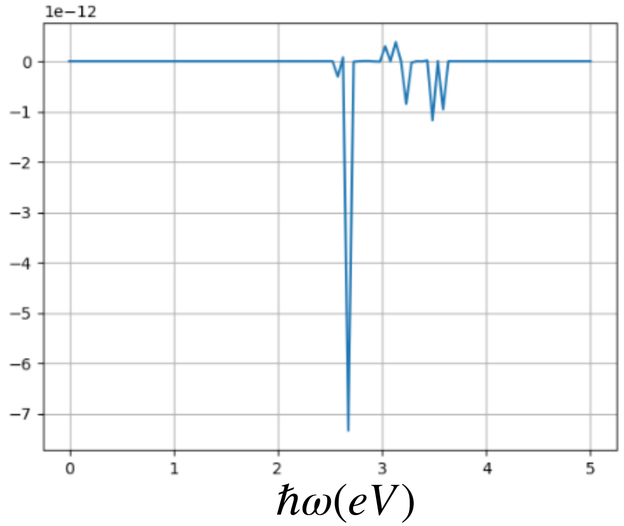
$\sigma_{xx}(\omega)$



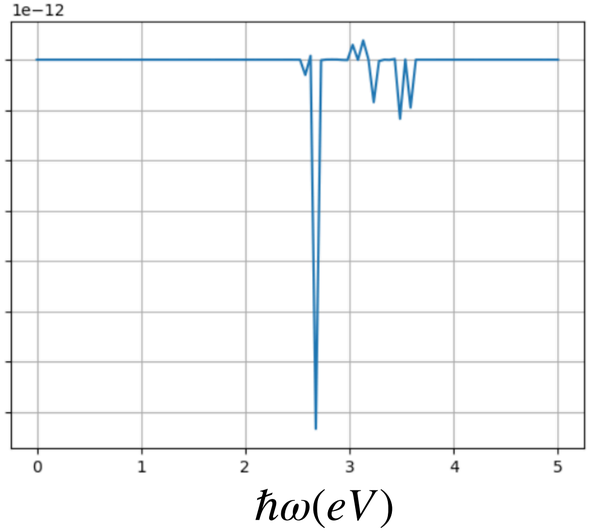
$\sigma_{yy}(\omega)$



$\sigma_{xy}(\omega)$

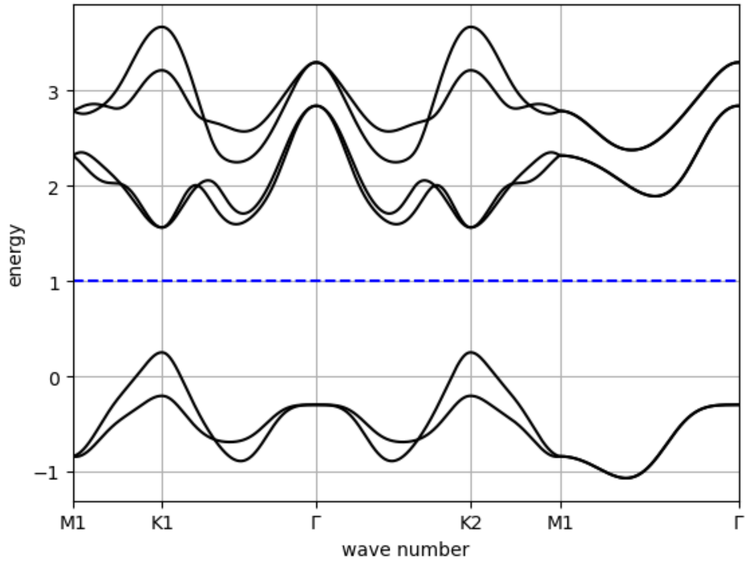


$\sigma_{yx}(\omega)$



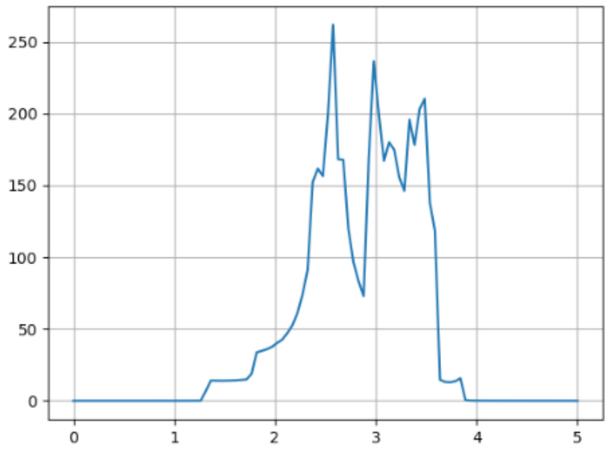
Optical conductivity of WSe_2

Chemical potential = 1



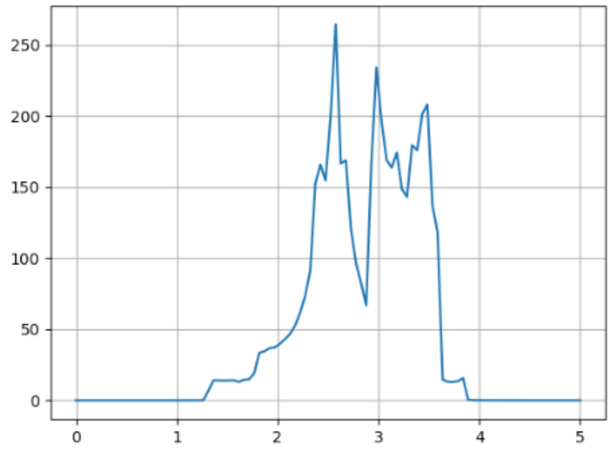
$\sigma_{xx}(\omega)$

$(e^2/\hbar)$



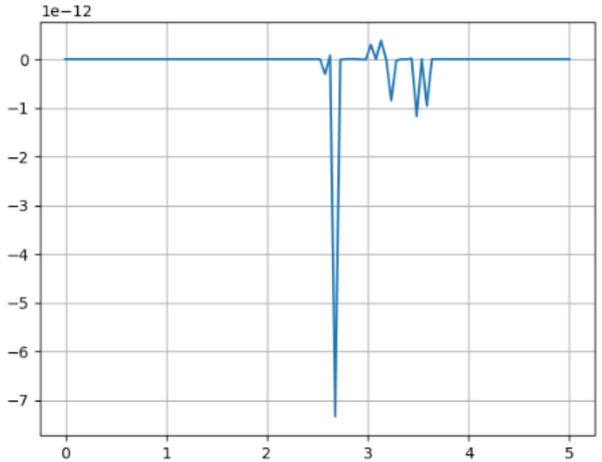
$\hbar\omega(eV)$

$\sigma_{yy}(\omega)$



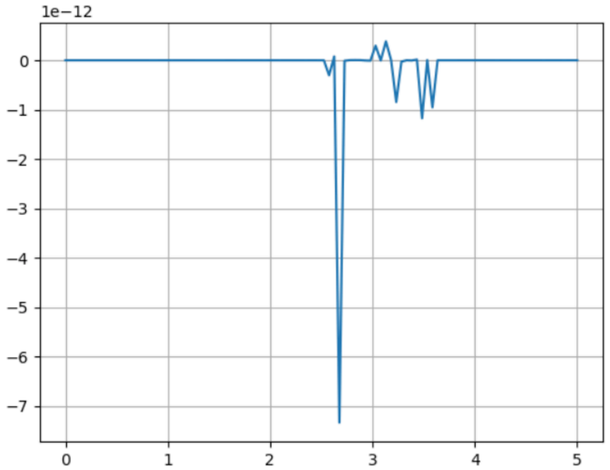
$\hbar\omega(eV)$

$\sigma_{xy}(\omega)$



$\hbar\omega(eV)$

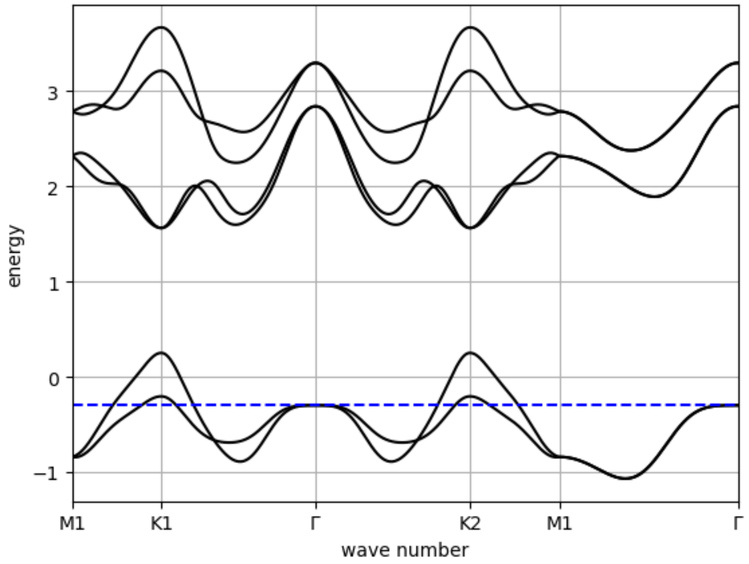
$\sigma_{yx}(\omega)$



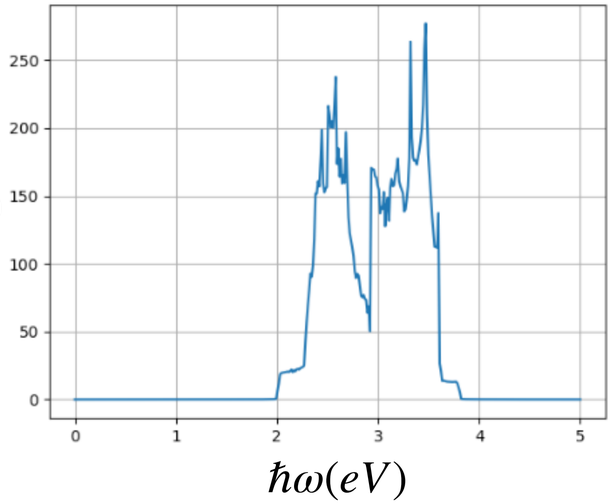
$\hbar\omega(eV)$

Optical conductivity of WSe_2

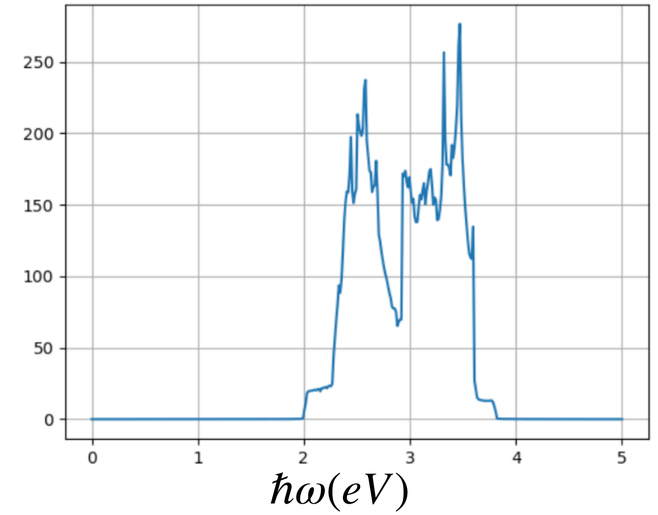
Chemical potential = -0.3



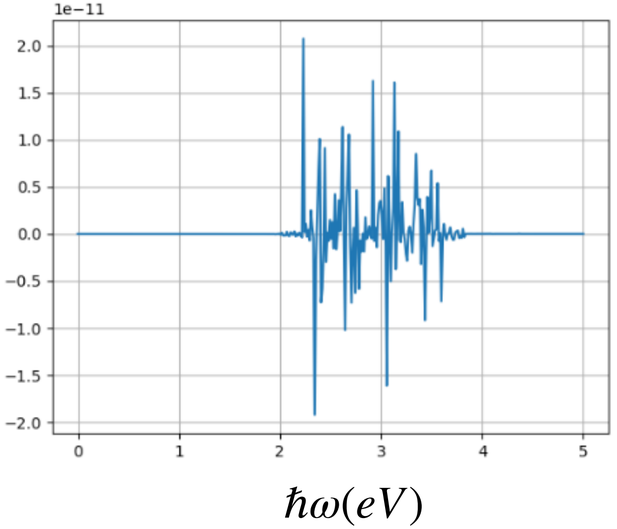
$\sigma_{xx}(\omega)$



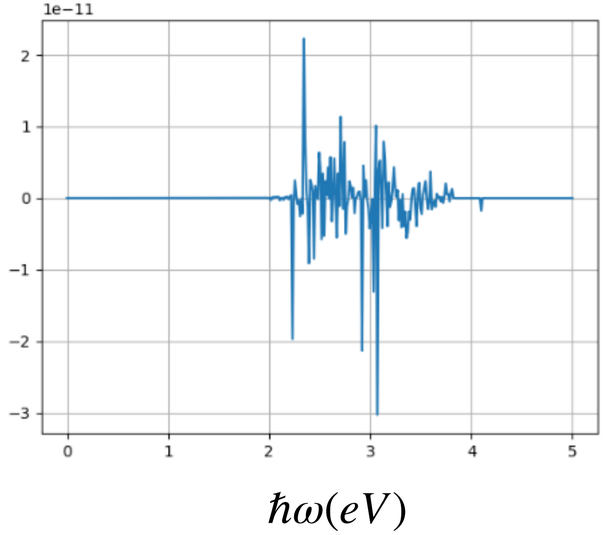
$\sigma_{yy}(\omega)$



$\sigma_{xy}(\omega)$



$\sigma_{yx}(\omega)$



Optical conductivity of WSe_2

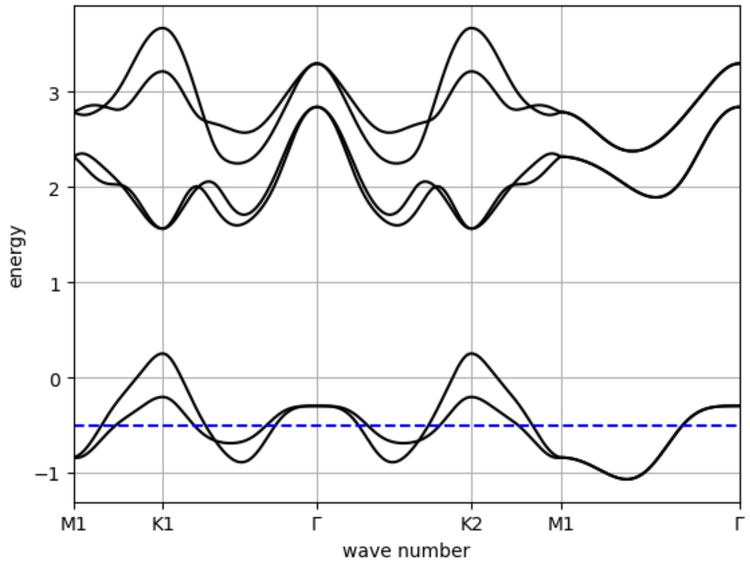
Chemical potential = -0.5

$\sigma_{xx}(\omega)$

$\sigma_{yy}(\omega)$

$(e^2/\hbar)$

Not yet



$\hbar\omega(eV)$

$\hbar\omega(eV)$

$\sigma_{xy}(\omega)$

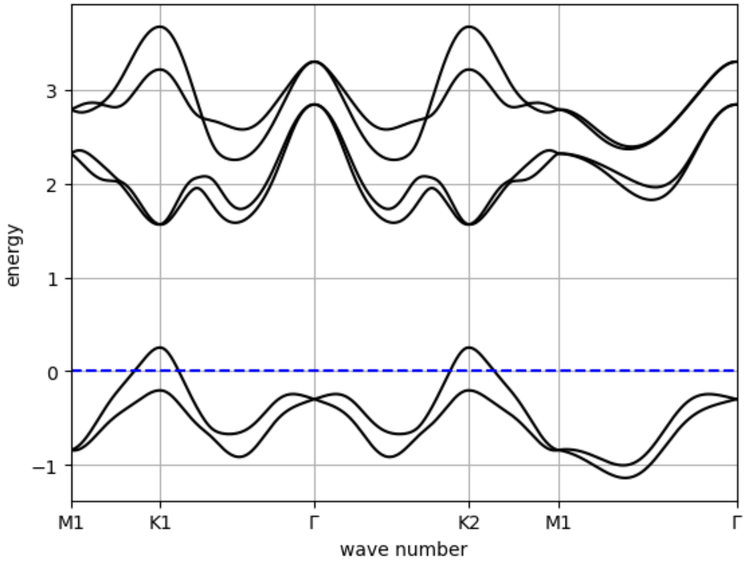
$\sigma_{yx}(\omega)$

$\hbar\omega(eV)$

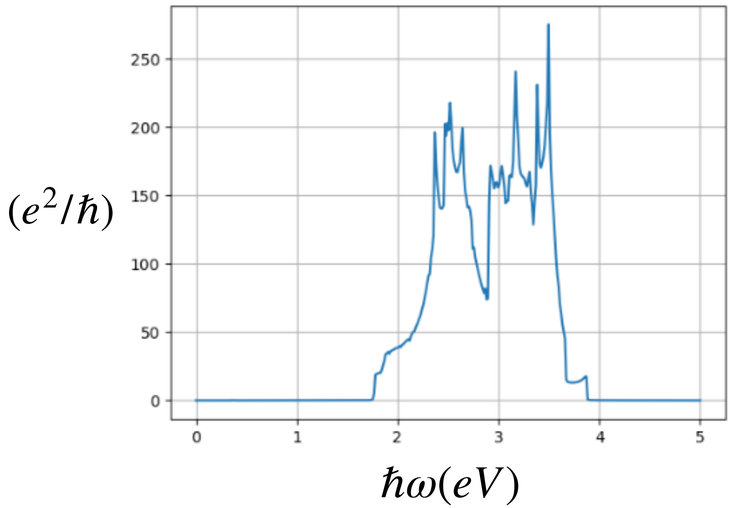
$\hbar\omega(eV)$

Optical conductivity of WSeTe

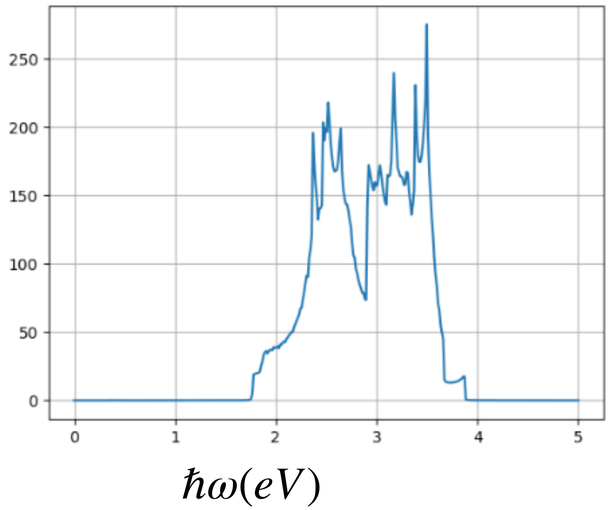
Chemical potential = 0



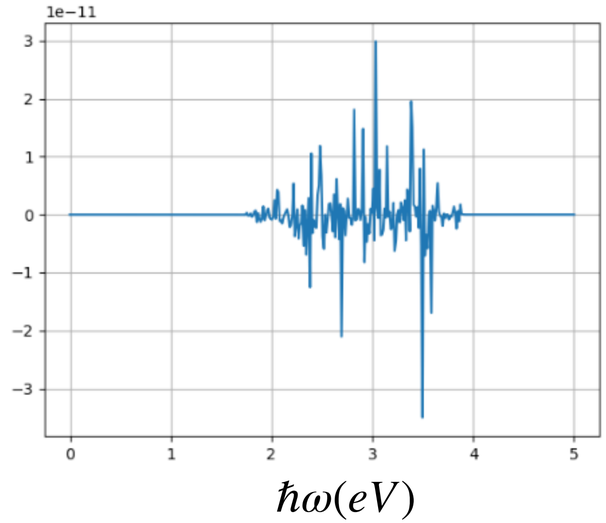
$\sigma_{xx}(\omega)$



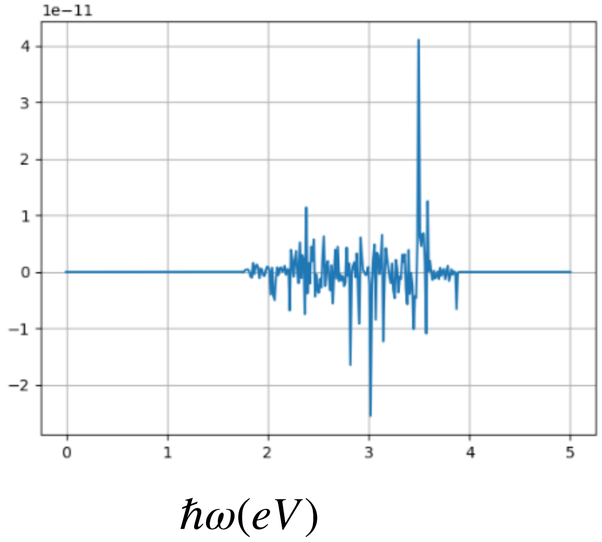
$\sigma_{yy}(\omega)$



$\sigma_{xy}(\omega)$

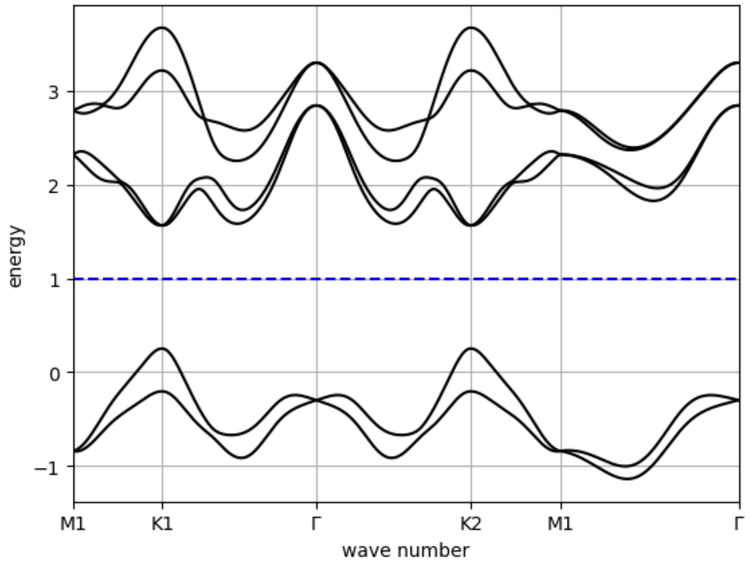


$\sigma_{yx}(\omega)$



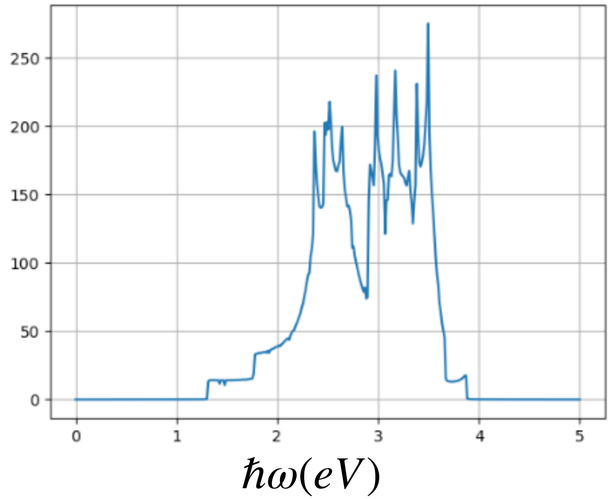
Optical conductivity of WSeTe

Chemical potential = 1



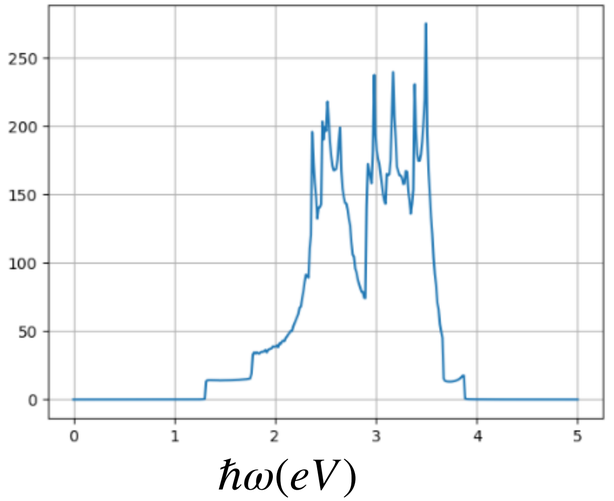
$\sigma_{xx}(\omega)$

$(e^2/\hbar)$



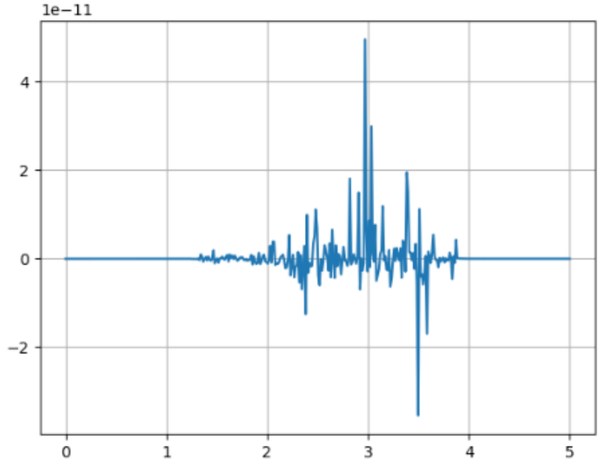
$\hbar\omega(eV)$

$\sigma_{yy}(\omega)$



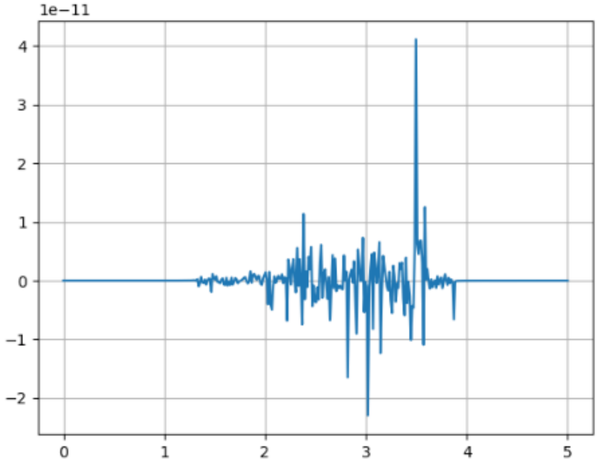
$\hbar\omega(eV)$

$\sigma_{xy}(\omega)$



$\hbar\omega(eV)$

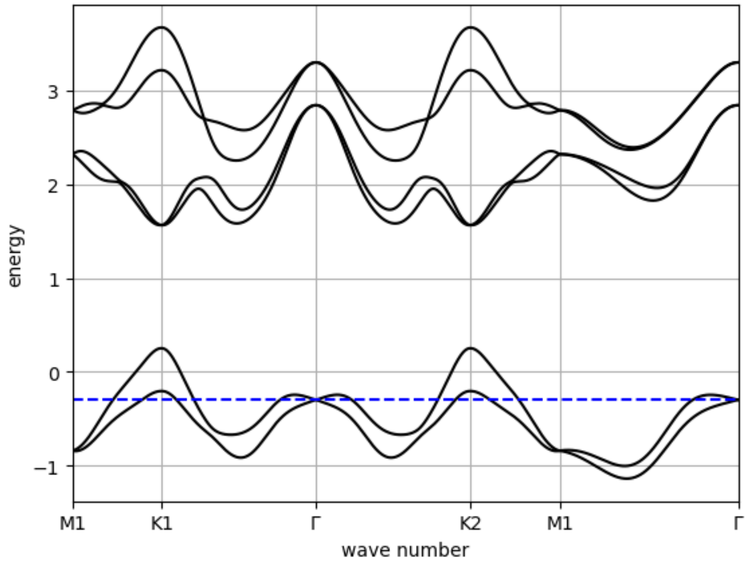
$\sigma_{yx}(\omega)$



$\hbar\omega(eV)$

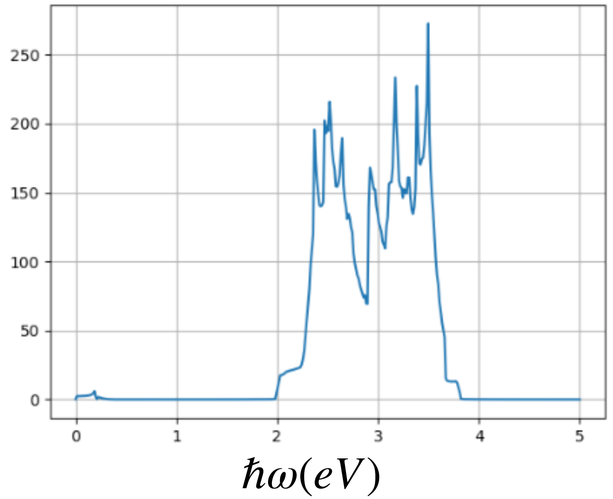
Optical conductivity of WSeTe

Chemical potential = -0.3



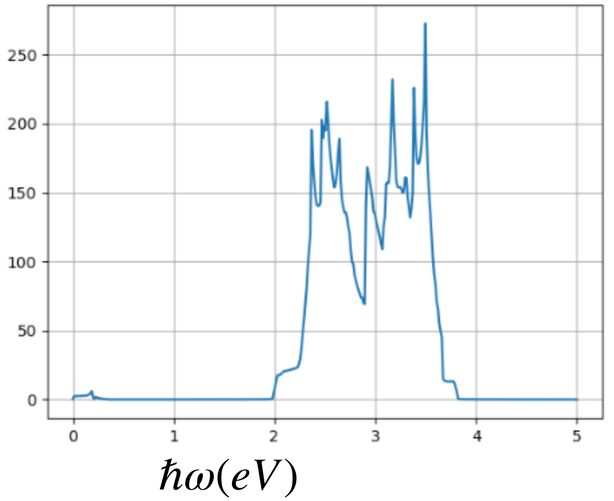
$\sigma_{xx}(\omega)$

$(e^2/\hbar)$



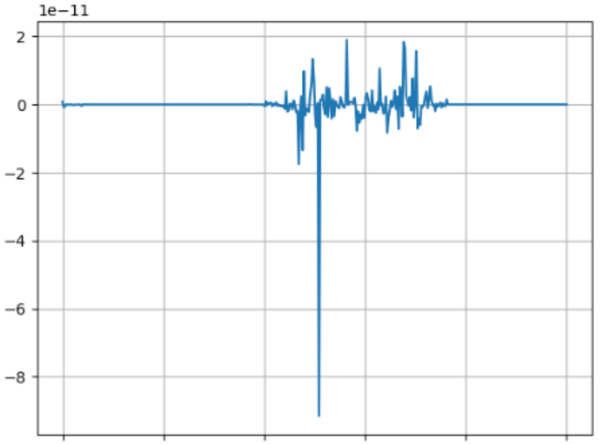
$\hbar\omega(eV)$

$\sigma_{yy}(\omega)$



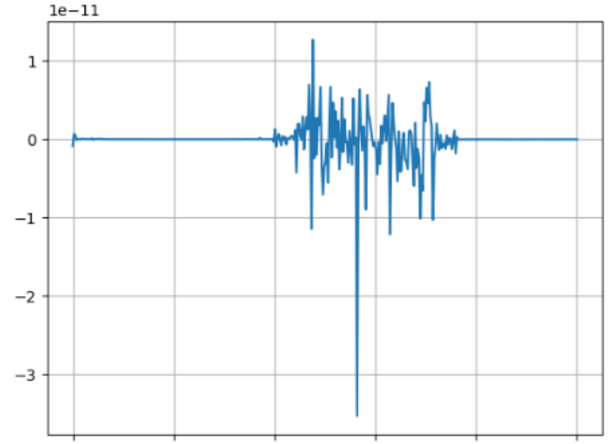
$\hbar\omega(eV)$

$\sigma_{xy}(\omega)$



$\hbar\omega(eV)$

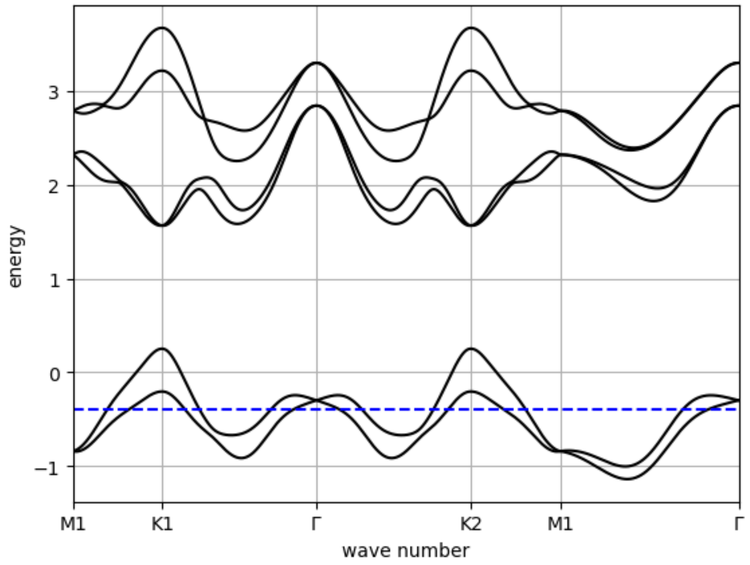
$\sigma_{yx}(\omega)$



$\hbar\omega(eV)$

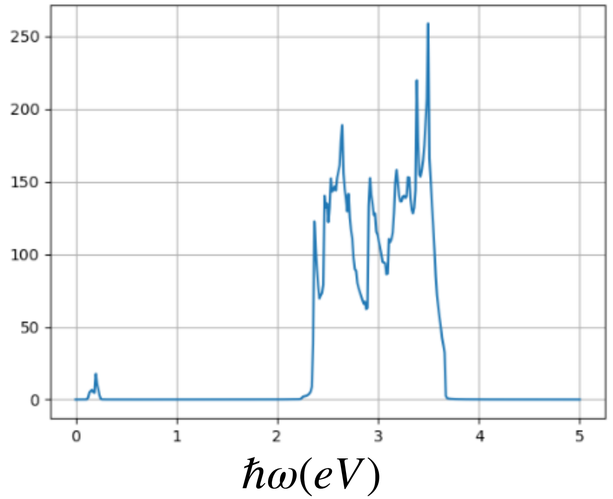
Optical conductivity of WSeTe

Chemical potential = -0.5

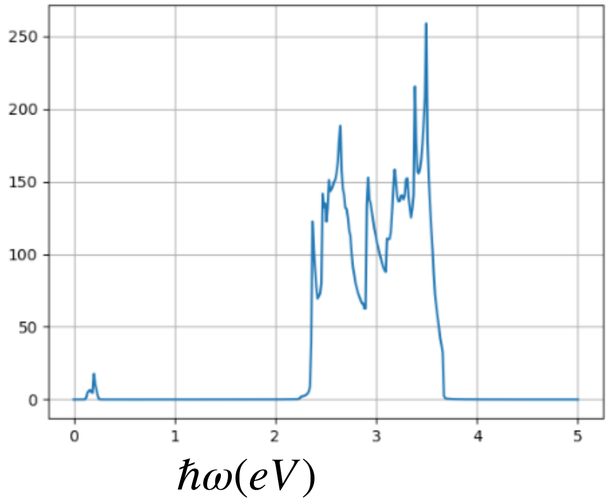


$(e^2/\hbar)$

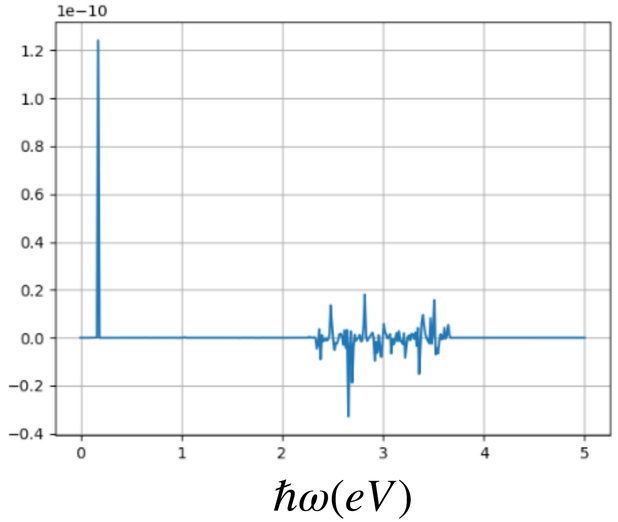
$\sigma_{xx}(\omega)$



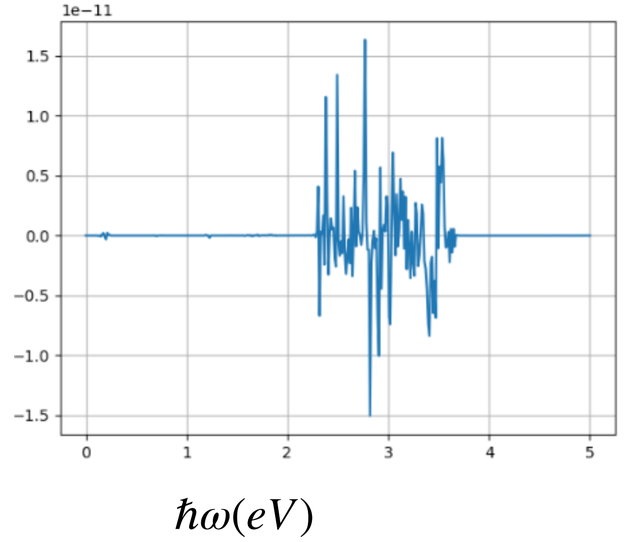
$\sigma_{yy}(\omega)$



$\sigma_{xy}(\omega)$



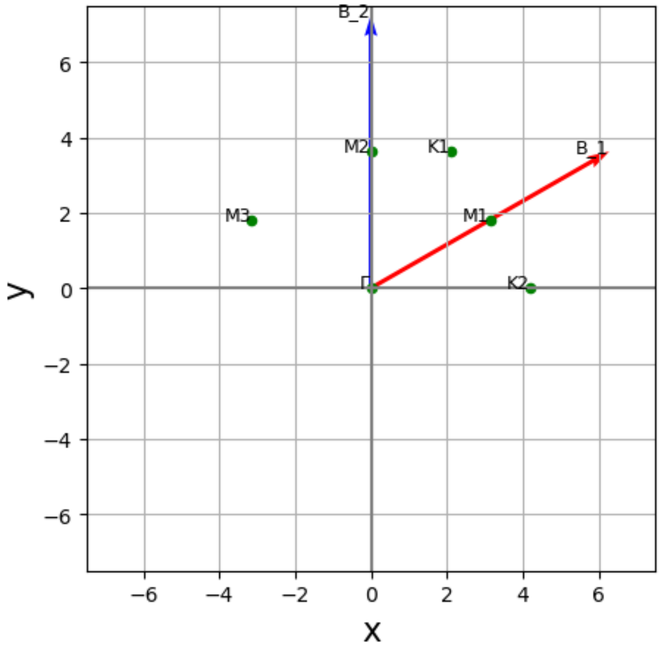
$\sigma_{yx}(\omega)$



Next

- Understand Rashba effect (theory)
- DFT and Wannier 90 (conductivity and berry curvature etc.)
- Spin hall conductivity(DC and AC)
- Insert bi-circular light
- Floque theory -> we can consider under AC field.
- Other Janus TMDCs

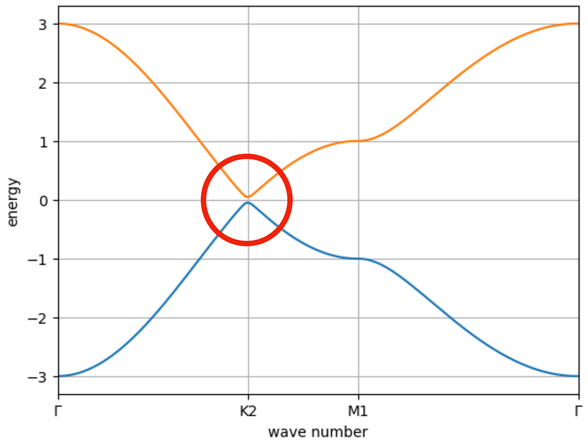
$$\Omega_{n,xy}^{s_z}(\boldsymbol{k}) = \hbar \sum_{m \neq n} \frac{-2\mathrm{Im}\left[\langle n\boldsymbol{k}|\hat{j}_x^z|m\boldsymbol{k}\rangle \langle m\boldsymbol{k}|\hat{v}_y|n\boldsymbol{k}\rangle\right]}{(E_{nk} - E_{mk})^2}$$



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

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

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

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

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

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

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

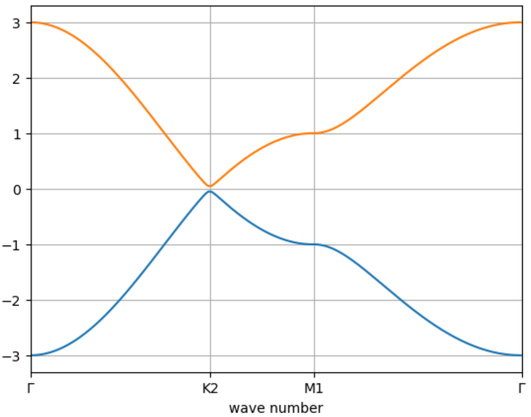
Berry phase in graphene

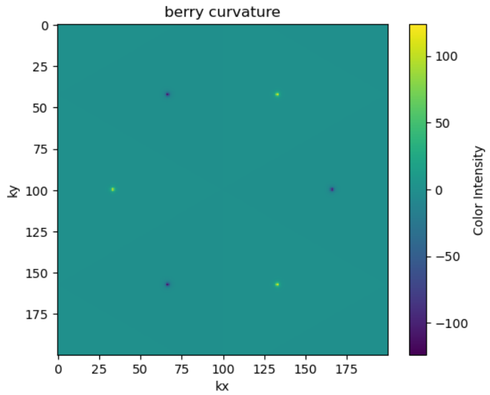
Numerical calculation

Berry curvature

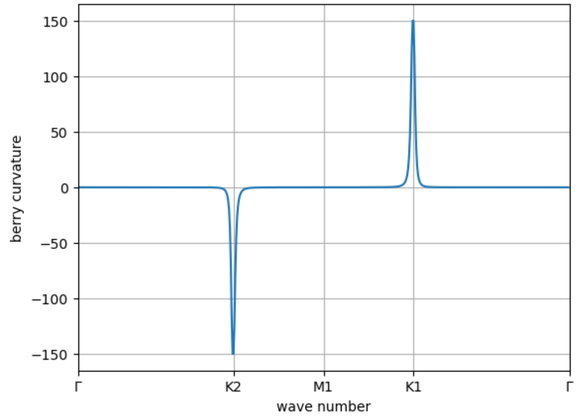
$$B_{n,z}(\boldsymbol{R}) = -2Im \sum_{(m \neq n)} \frac{\langle \phi_n(\boldsymbol{R}) | \frac{\partial \hat{H}(\boldsymbol{R})}{\partial R_x} | \phi_m(\boldsymbol{R}) \rangle \langle \phi_m(\boldsymbol{R}) | \frac{\partial \hat{H}(\boldsymbol{R})}{\partial R_y} | \phi_n(\boldsymbol{R}) \rangle}{(E_n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

High band

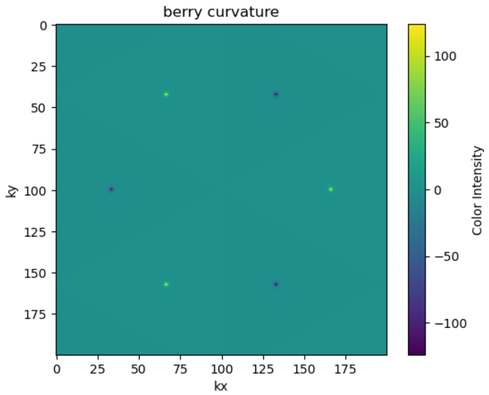




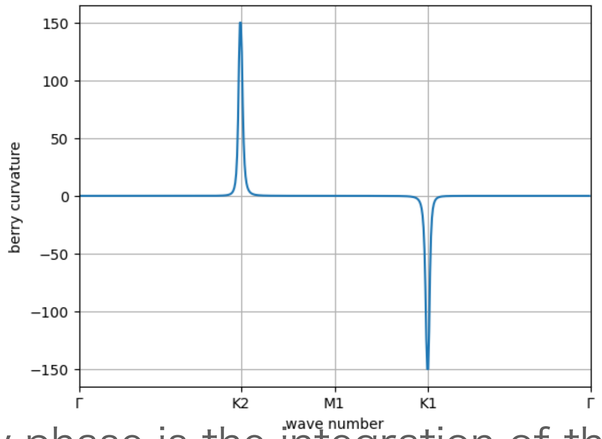
BZ



Low band



BZ



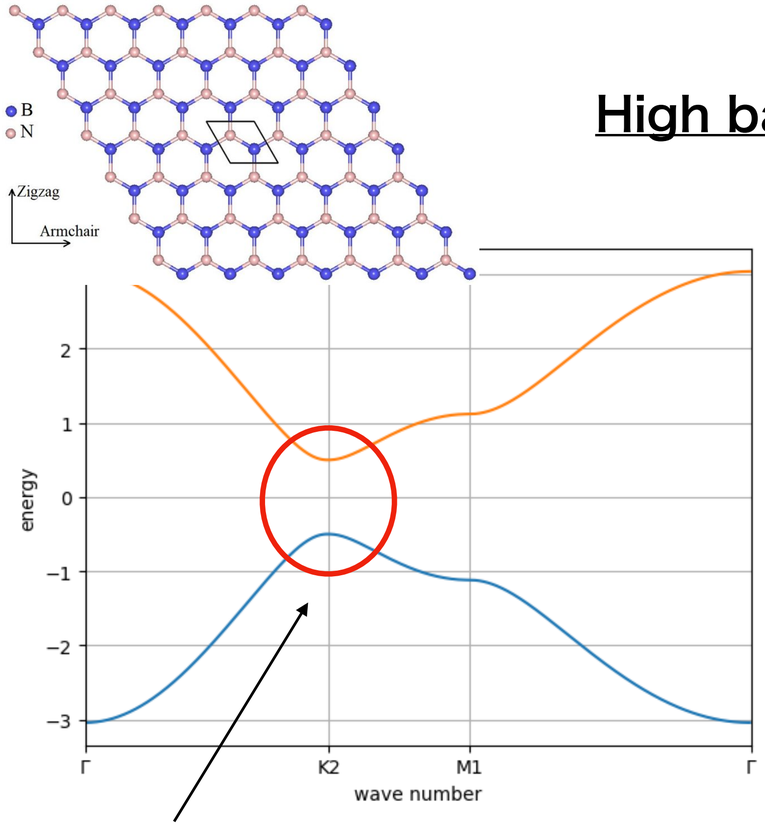
Berry curvature is 0 all over the BZ

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

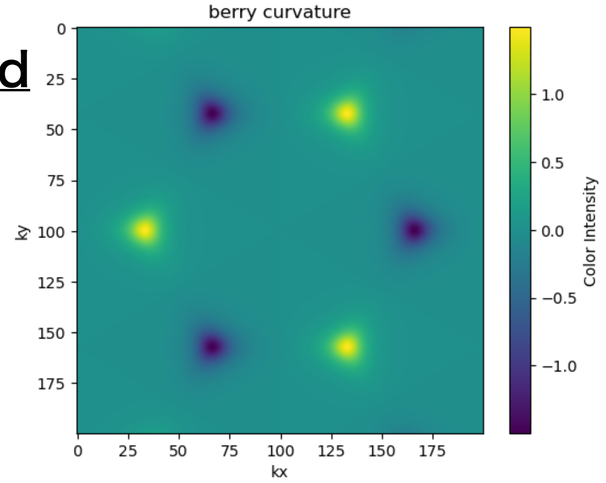
Breaking Inversion symmetry

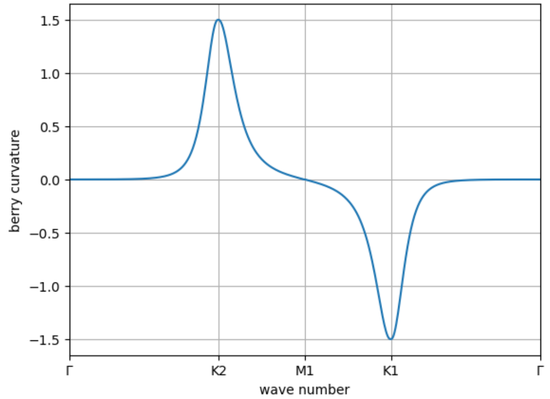


Open energy gap

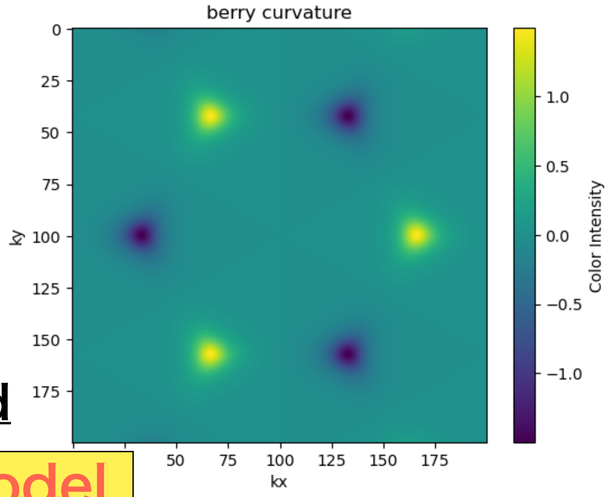
Berry curvature

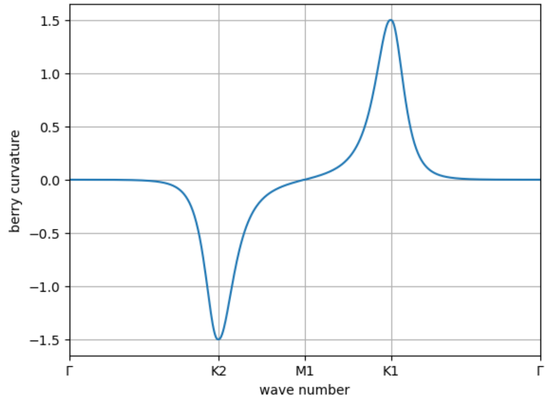
High band





Low band

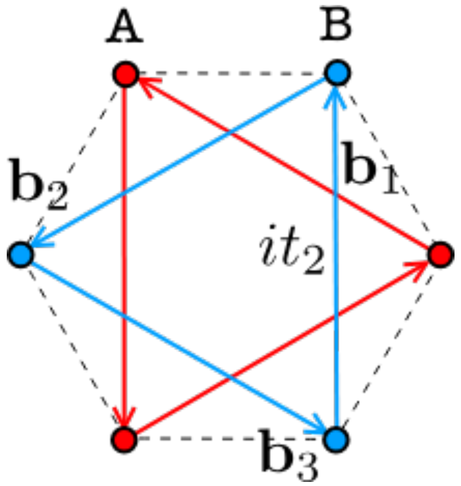


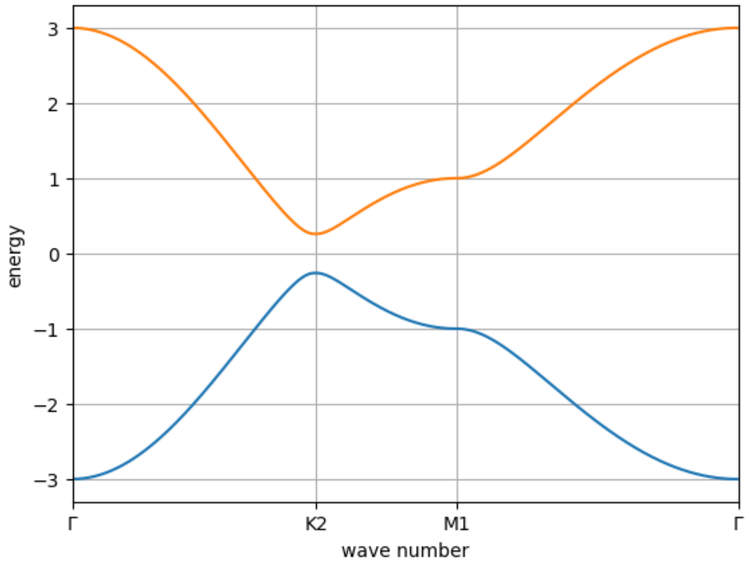


BC is odd-function in h-BN model

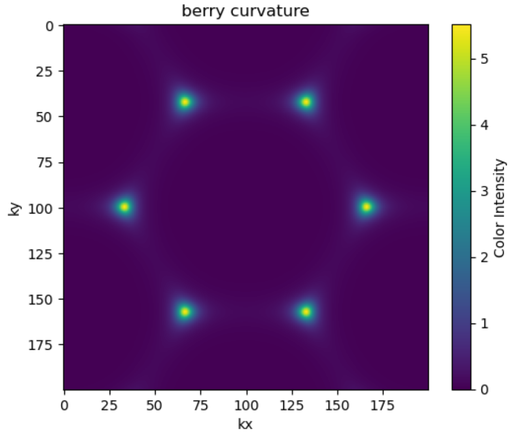
Berry phase in Haldane model

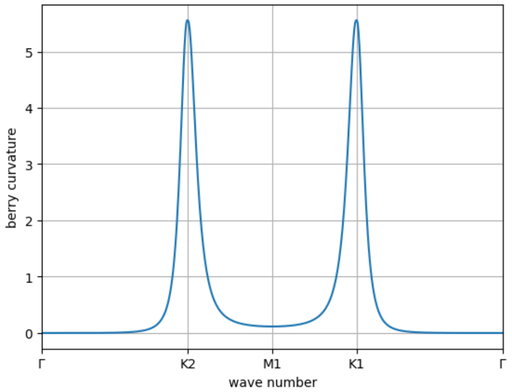
Breaking Time reversal symmetry

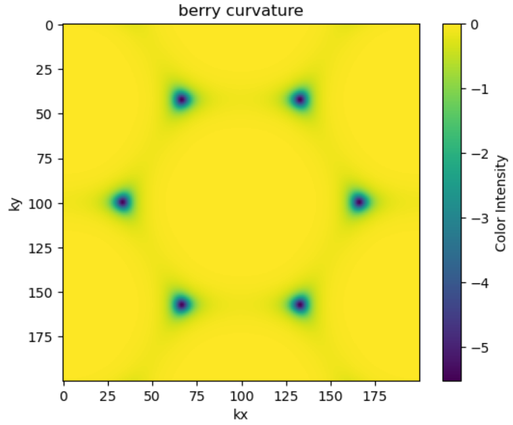


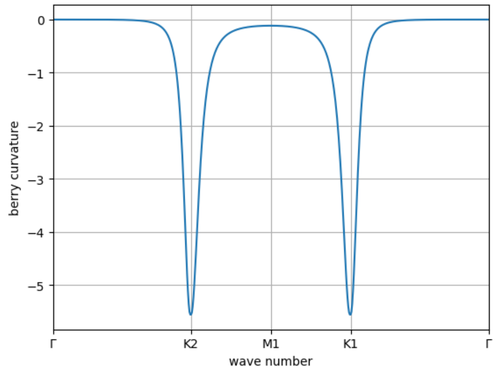


Berry curvature









BC is even-function in Haldane model