◆ Goal:

Construction arbitrary dimension kp Hamiltonian, solve band structure, calculation of Berry curvature and first Chern number.

◆ Berry curvature calculation:

$$\overrightarrow{\Omega}_{uv}^{m}(\overrightarrow{R}) = i \sum_{n \neq m} \frac{\langle m \mid \nabla_{R_{u}} \mathbf{H} \mid n \rangle \langle n \mid \nabla_{R_{v}} \mathbf{H} \mid m \rangle - \langle m \mid \nabla_{R_{v}} \mathbf{H} \mid n \rangle \langle n \mid \nabla_{R_{u}} \mathbf{H} \mid m \rangle}{(\varepsilon_{m} - \varepsilon_{n})^{2}}$$

$$C_{1,n} = \int_{B.Z.} \overrightarrow{\Omega}_n(\overrightarrow{R}) \frac{d\overrightarrow{R}}{(2\pi)^{d-1}}$$

Ref: Rev. Mod. Phys. 82, 1959 (2010)

Note:

- 1, Dimension of Hamiltonian is controlled by Kronecker tensor product of Pauli matrix representing different d.o.f.: sublattice, orbital, valley, spin...; see the difference between two_band and four_band
- 2, In running the code, we need to change N, H, Hx, Hy and the band you concern;