MSc PROJECT – FINAL PRESENTATION

TOPOLOGICAL HALL EFFECT DUE TO ITINERANT ELECTRON IN HONEYCOMB SKYRMION CRYSTAL

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CONTENT

1) Magnetic Skrmions

Definition of magnetic skyrmions, classification, anatomy & topology of skyrmions, Triple Q state (sKx). Problem statement – Electronic properties of sKx.

2) Adiabatic Berry Phase

Berry phase, Berry connection, Berry curvature, Adiabatic theorem (time evolution of a quantum state).

3) Quantum Hall effect

Velocity and Berry curvature in QHE, Hall conductance & TKNN relation.

4) Results & discussion

Band structure and Hall conductivity in finite Hund's coupling limit, Large coupling limit, Comparison with zero field band structure, Onsager Quantization scheme, Skyrmion size effects.

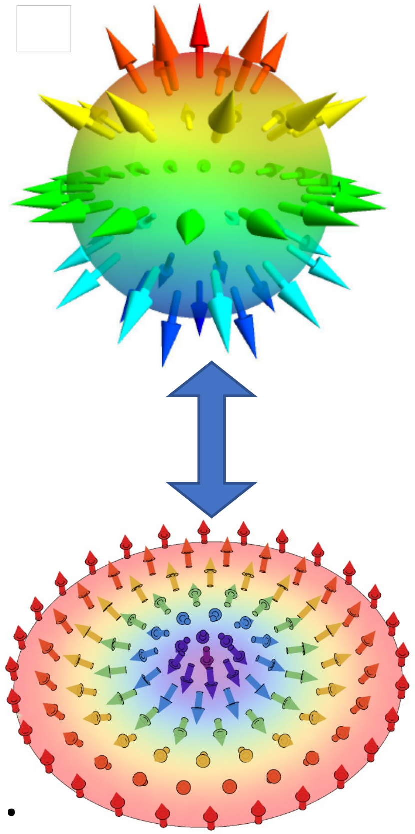
5) Conclusion & Future work

Rashba and Dresselhaus effects on skyrmion and anti skyrmion.

MAGNETIC SKYRMIONS (Topological defects)

Magnetic Quasiparticles (or) Topological Excitations in field of magnetic moments.

Stereographic Projection ($2D \rightarrow 3D$) → Non – trivial real space topology (Topological protection)



$$N_{sk} \stackrel{\text{def}}{=} \frac{1}{4\pi} \int n(\vec{r}).\left\{\frac{\partial \vec{n}(\vec{r})}{\partial x} \times \frac{\partial \vec{n}(\vec{r})}{\partial y}\right\} d^2 r \quad , (N_{sk} \in \mathrm{Z})$$

$$N_{sk} = p\,.m$$

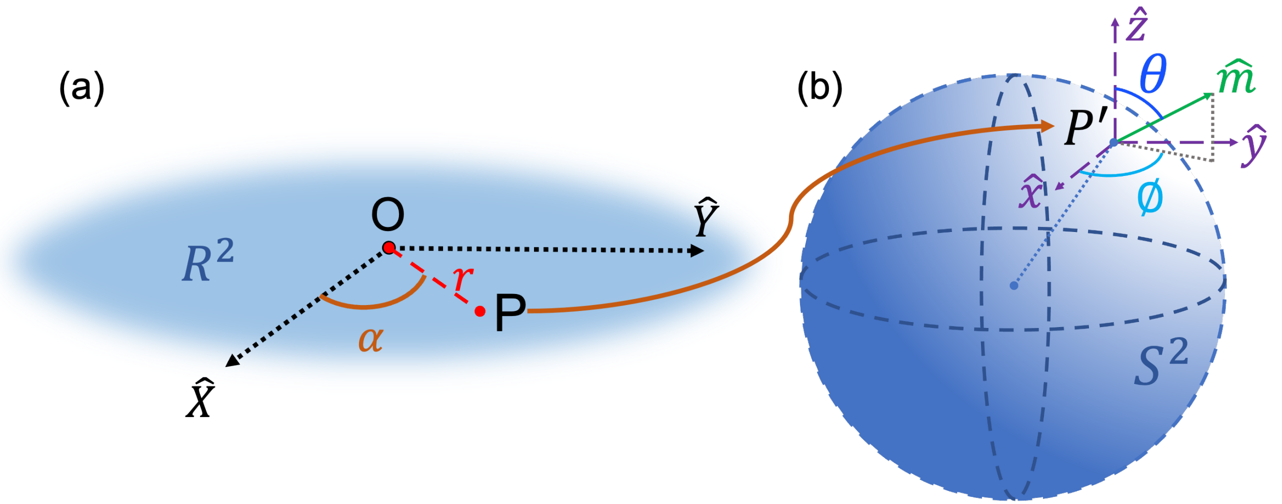
Polarity, $p \rightarrow$ indicates sign of central spin.

Vorticity, $m \rightarrow$ quantifies in-plane rotation of $n(\vec{r})$ (winding number).

Helicity, $\gamma \rightarrow$ twist around central spin.

CLASSIFICATION OF SKYRMION (N_{sk}, m, γ)

$$\hat{m} = (\sin\theta(r)\cos\varphi(\alpha), \sin\theta(r)\sin\varphi(\alpha), \cos\theta(r))$$

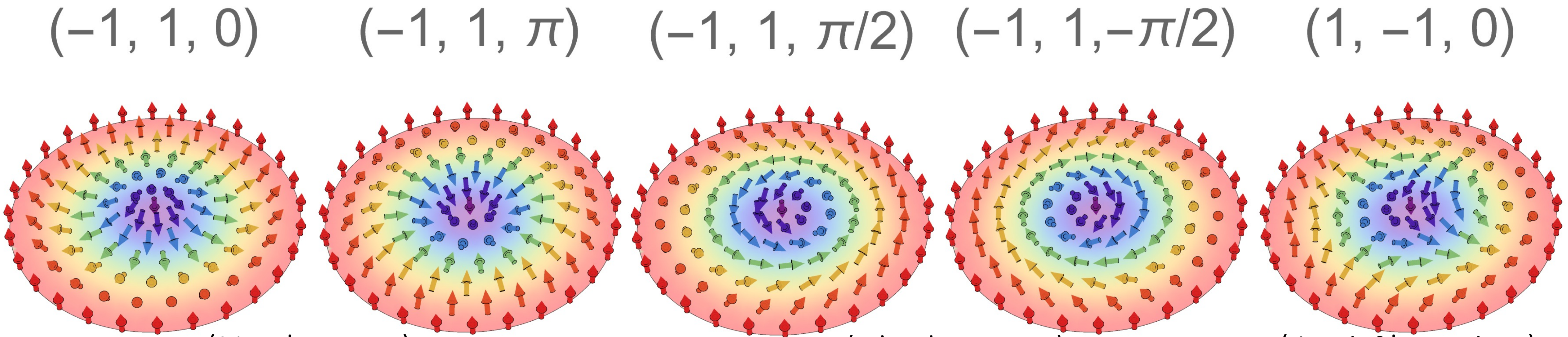


- ❖ θ(r) - changes from 0 in the center to π at the edges (vice versa)

  $\theta(r) = \pi\left[1 - \frac{r}{\lambda}\right]$ for N_{sk} = -1

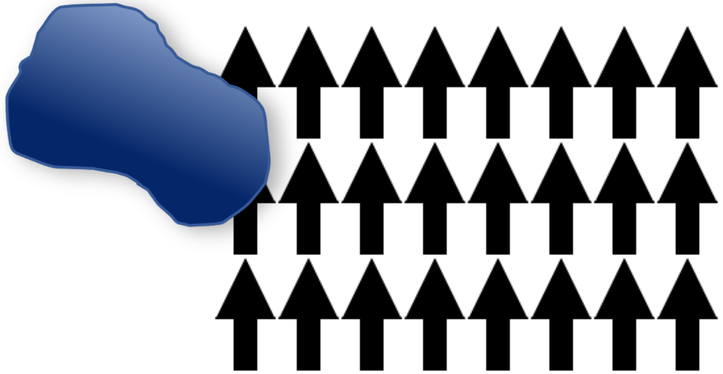
- ❖ $\varphi(\alpha)$ - Linear variation model

  $\varphi(\alpha) = \mathrm{m}\,\alpha + \gamma$



(Neel - type) (Bloch - type) (Anti-Skyrmion)

SKYRMION ANATOMY & TOPOLOGY

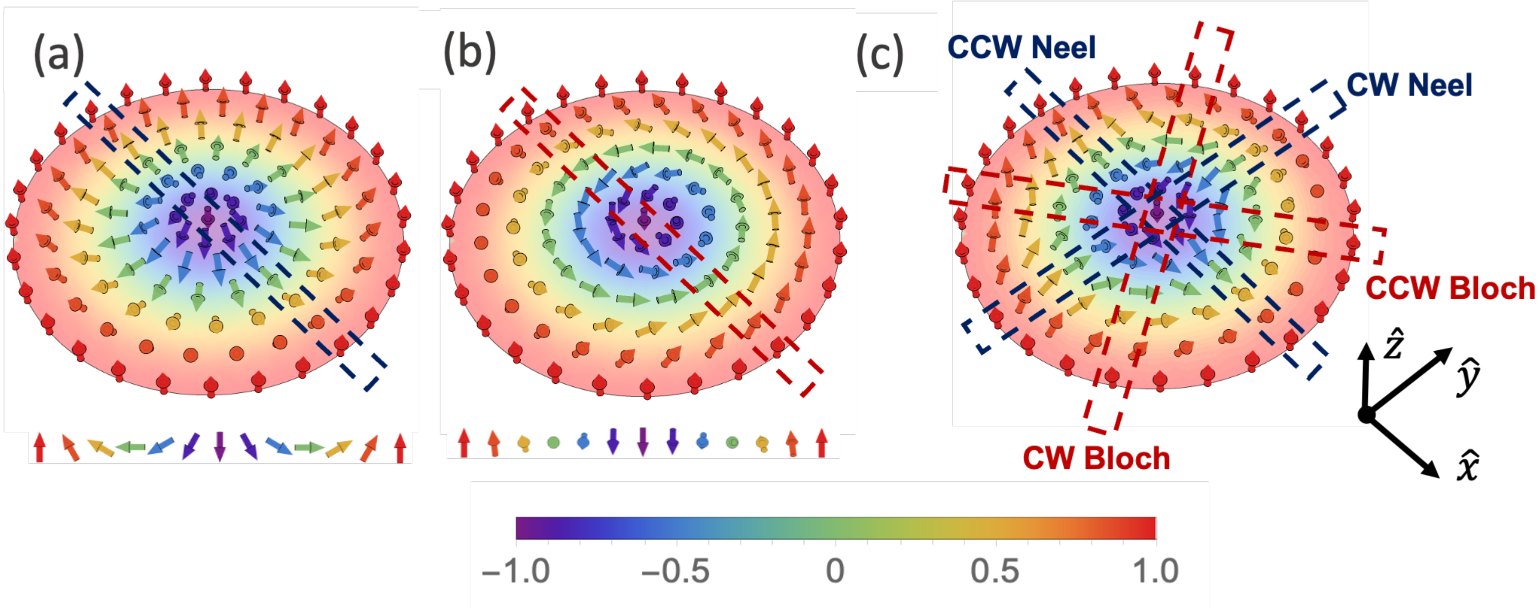


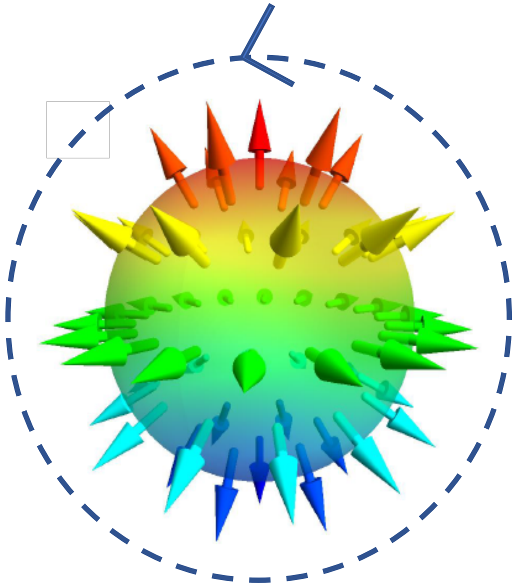
Topological number = 0

Topological number = 1

Real space → Winding number

Reciprocal space → Chern number





Winding number = 1

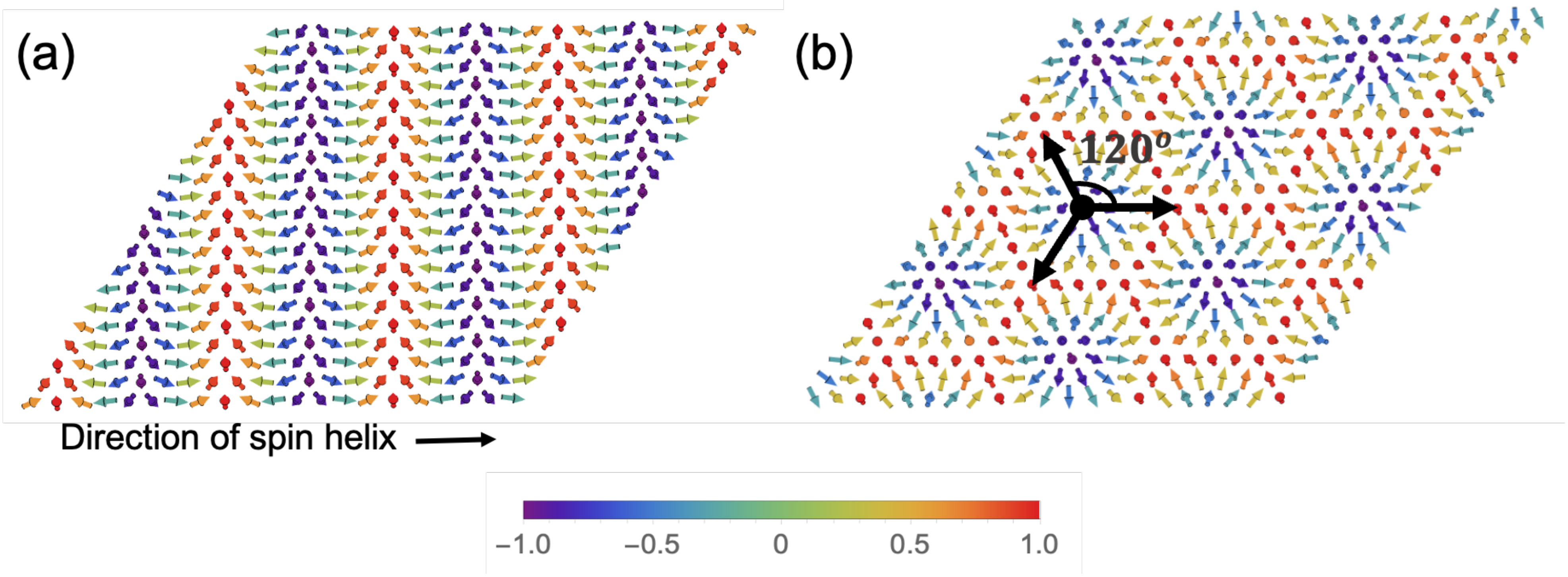
Triple Q SkX state

Superposition of 3 spin helices at 120 degree directions.

$$\widetilde{m}_{xy}(\boldsymbol{r}) = \sum_{j=1}^{3} \sin(\boldsymbol{Q}_i \cdot \boldsymbol{r} + \theta_j)\, \boldsymbol{e}_j,$$
$$\widetilde{m}_{z}(\boldsymbol{r}) = \sum_{j=1}^{3} \cos(\boldsymbol{Q}_i \cdot \boldsymbol{r} + \theta_j) + m_0,$$

Conditions,

$$\sum_{i=1}^{3} \hat{e}_i = 0 \qquad \sum_{i=1}^{3} \theta_i = 0\ (or)\ \pi$$

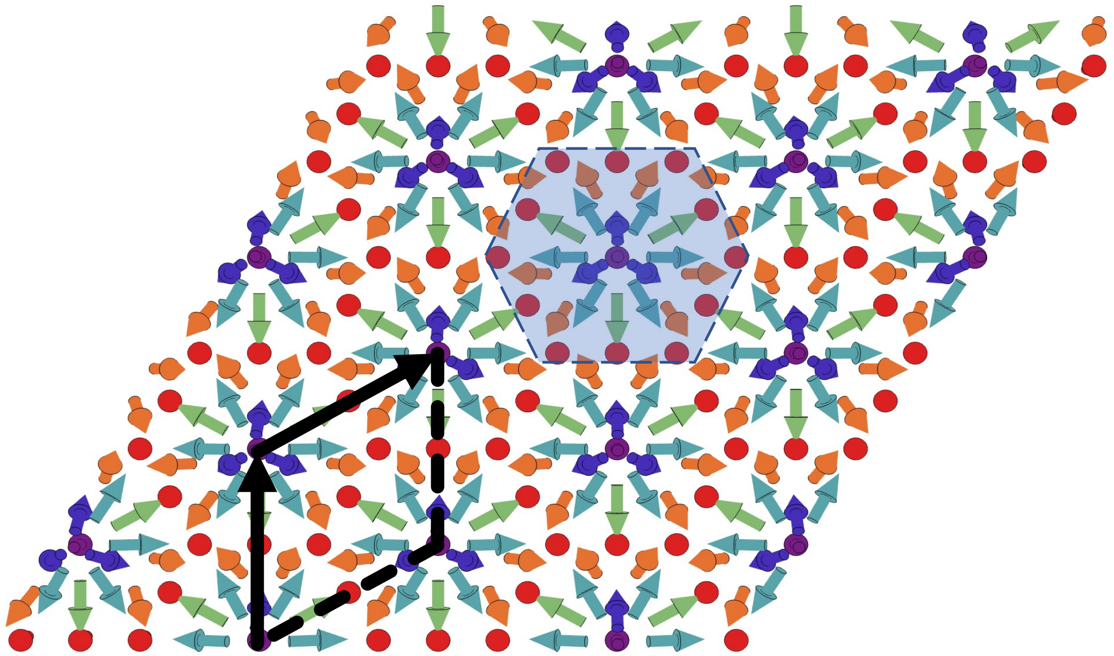


T. Okubo, S. Chung, and H. Kawamura, Phys. Rev. Lett. 108,017206 (2012).

HONEYCOMB LATTICE

Triple Q SkX state

$$\widetilde{m}_{xy}(\boldsymbol{r}) = \sum_{j=1}^{3} \sin(\boldsymbol{Q}_i \cdot \boldsymbol{r} + \theta_j)\, \boldsymbol{e}_j,$$
$$\widetilde{m}_z(\boldsymbol{r}) = \sum_{j=1}^{3} \cos(\boldsymbol{Q}_i \cdot \boldsymbol{r} + \theta_j) + m_0,$$

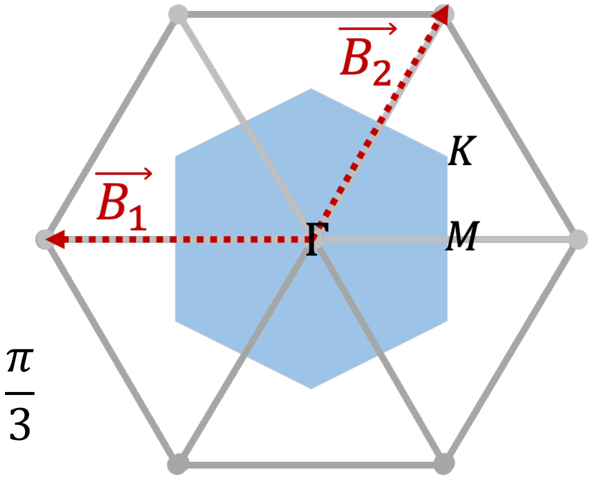


24 sites unit cell

Conditions,

$$\sum_{i=1}^{3} \hat{e}_i = 0 \qquad \sum_{i=1}^{3} \theta_i = \pi$$

Q_i' ‘s are the Reciprocal lattice vectors with 120^o separation.



$$Q = \left\{\left(\frac{2\pi}{3}, 0\right), \left(\frac{-\pi}{3}, \frac{\pi}{\sqrt{3}}\right), \left(\frac{-\pi}{3}, \frac{-\pi}{\sqrt{3}}\right)\right\} \quad \hat{e} = \left\{(1,0), \left(\frac{-1}{2}, \frac{\sqrt{3}}{2}\right), \left(\frac{-1}{2}, \frac{-\sqrt{3}}{2}\right)\right\} \quad \theta_i = \frac{\pi}{3}$$

GÖBEL, MOOK, HENK, AND MERTIG, PHYSICAL REVIEW B 96, 060406(R) (2017)

ELECTRONIC PROPERTIES OF A SkX

Free electron Hamiltonian coupled with the spin texture modelled by **Hund's coupling**

$$\hat{\mathcal{H}} = \sum_{ij} t_{ij}\hat{C}_i^{\dagger}\hat{C}_j - J\sum_i \vec{\boldsymbol{n}}.\,(\hat{C}_i^{\dagger}\boldsymbol{\sigma}\hat{C}_i)$$

In itinerant electrons perspective: $\hat{U}_{\boldsymbol{i}}^{\dagger}(\vec{\boldsymbol{n}}.\vec{\boldsymbol{\sigma}})\hat{U}_i = \sigma_z$

$$\begin{bmatrix} \cos\left(\frac{\theta}{2}\right) & e^{-i\varphi}\sin\left(\frac{\theta}{2}\right) \\ e^{i\varphi}\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{bmatrix} \begin{bmatrix} cos\theta & e^{-i\varphi}sin\theta \\ e^{i\varphi}sin\theta & -cos\theta \end{bmatrix} \begin{bmatrix} \underbrace{\begin{matrix} \cos\left(\frac{\theta}{2}\right) \\ e^{i\varphi}\sin\left(\frac{\theta}{2}\right) \end{matrix}}_{|\chi^{\uparrow}>} & \underbrace{\begin{matrix} e^{-i\varphi}\sin\left(\frac{\theta}{2}\right) \\ \cos\left(\frac{\theta}{2}\right) \end{matrix}}_{|\chi^{\downarrow}>} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\hat{C}_i = \hat{U}\hat{d}_i \longrightarrow \hat{\mathcal{H}} = \sum_{ij} t_{ij}\hat{U}_{\boldsymbol{i}}^{\dagger}\hat{U}_{\boldsymbol{j}}\hat{d}_i^{\dagger}\hat{d}_j - J\sum_i (\hat{d}_i^{\dagger}\sigma_z\hat{d}_i)$$

K. Hamamoto, M. Ezawa, and N. Nagaosa, Phys. Rev. B 92,115417 (2015).

$$\hat{U}_i^{\dagger}\hat{U}_j = \begin{bmatrix} \langle \chi_i^{\uparrow} | \chi_j^{\uparrow} \rangle & \langle \chi_i^{\uparrow} | \chi_j^{\downarrow} \rangle \\ \langle \chi_i^{\downarrow} | \chi_j^{\uparrow} \rangle & \langle \chi_i^{\downarrow} | \chi_j^{\downarrow} \rangle \end{bmatrix}$$

$$t_{ij}^{eff} = t_{ij} \left\langle \chi_i^{\uparrow} \middle| \chi_j^{\uparrow} \right\rangle$$
$$= t_{ij} \left(\cos\left(\frac{\theta_i}{2}\right) \cos\left(\frac{\theta_j}{2}\right) + \sin\left(\frac{\theta_i}{2}\right) \sin\left(\frac{\theta_j}{2}\right) e^{-i(\phi_i - \phi_j)} \right)$$

$$\hat{\mathcal{H}}_{eff} = \sum_{ij} t_{eff} \hat{d}_i^{\dagger} \hat{d}_j$$
$$t_{eff} = t_{ij} \hat{U}_i^{\dagger} \hat{U}_j = t_{ij} \langle \chi_i | \chi_j \rangle$$

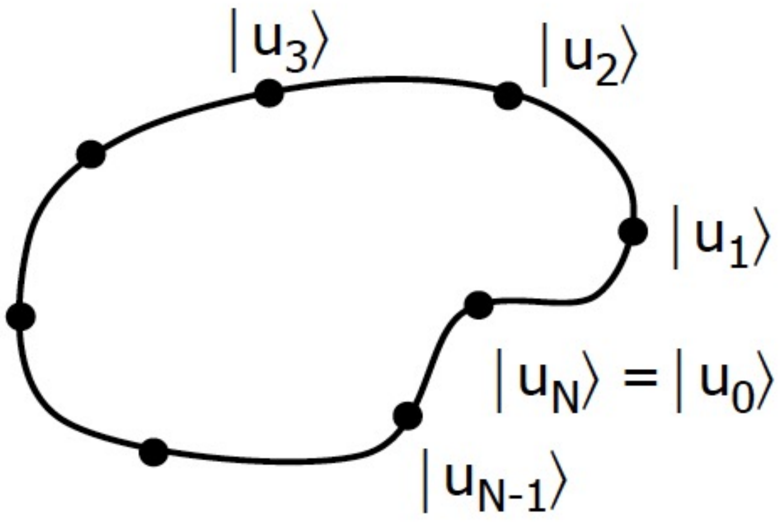
$$t_{ij}^{eff} = t_{ij} e^{i a_{ij}} \cos\left(\frac{\theta_{ij}}{2}\right) = t_{\vec{A}\neq 0} = t_{\vec{A}\neq 0} \exp\left\{ \frac{ie}{\hbar} \int_i^j \vec{A}.d\vec{r} \right\}$$

Hunds coupling is like an **effective magnetic field** due to the skyrmion topology

IQHE due to uniform strong magnetic field (attains extra **phase due to geometry**)

BERRY PHASE (“Geometric Phase”)

Berry phase : Phase angle that describes the global phase evolution of a complex vector as it is carried around a path in its vector space. ($0 \leq \boldsymbol{\varphi} < \boldsymbol{2\pi}$)



$$\boldsymbol{\varphi} \stackrel{\text{def}}{=} -\boldsymbol{Im}\left\{\sum_{n=0}^{N-1} \boldsymbol{Ln}(\langle \boldsymbol{u_n} | \boldsymbol{u_{n+1}} \rangle)\right\}$$

E.g. : (Spin – ½ particle in uniform B)

$$|\uparrow_{\hat{\mathbf{n}}}\rangle = \begin{pmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{pmatrix}$$

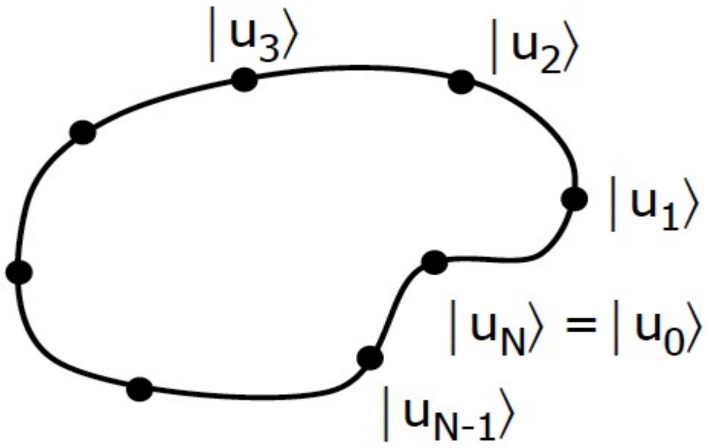
Assume discrete states along $\hat{x}$, $\hat{y}$ & $\hat{z}$ directions,

$$\hat{x} \rightarrow \hat{y} \rightarrow \hat{z} \rightarrow \hat{x}$$

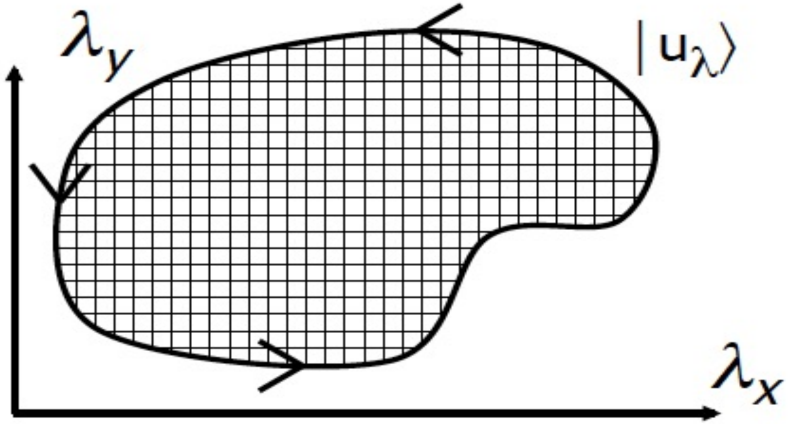
$$|\uparrow_x\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad |\uparrow_y\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix} \quad |\uparrow_z\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$\varphi = -Im\,\{Ln(1\,(1+i)\,1)\} = -\frac{\pi}{4}$$

BERRY PHASE (continuous formulation)



$\boldsymbol{\lambda}$ is some parameter
in physics it is $\boldsymbol{k}$



$$\varphi = -Im\left\{\sum_{n=0}^{N-1} Ln(\langle u_n|u_{n+1}\rangle)\right\}$$

$$\varphi \equiv -Im\left\{\oint\langle u_\lambda|\vec{\nabla_\lambda}|u_\lambda\rangle . d\vec{\lambda}\right\}$$

$$\boldsymbol{\varphi = \oint\langle u_\lambda|i\vec{\nabla_\lambda}|u_\lambda\rangle . d\vec{\lambda}}$$

$$\begin{aligned}\ln\langle u_\lambda|u_{\lambda+d\lambda}\rangle &= \ln\langle u_\lambda|\left(|u_\lambda\rangle + d\lambda\,\frac{d|u_\lambda\rangle}{d\lambda} + \ldots\right) \\ &= \ln(1 + d\lambda\,\langle u_\lambda|\partial_\lambda u_\lambda\rangle + \ldots) \\ &= d\lambda\,\langle u_\lambda|\partial_\lambda u_\lambda\rangle + \ldots\end{aligned}$$

BERRY CURVATURE

Berry curvature, $\Omega(\vec{\lambda})$ is simply defined as the **Berry phase per unit area** in parameter space (reciprocal space).

$$\phi = \oint_C \mathbf{A} \cdot d\boldsymbol{\lambda} = \int_S \boldsymbol{\Omega} \cdot \hat{\mathbf{n}}\, dS = \int_S \boldsymbol{\Omega} \cdot d\mathbf{S}$$

In Vector notations, $\vec{\Omega}(\vec{\lambda}) \overset{\text{def}}{=} \overrightarrow{\nabla_{\boldsymbol{\lambda}}} \times \vec{A}$

ANALOGOUS TO EMT

Berry connection ⟺ Magnetic vector potential
Berry curvature ⟺ Magnetic field

Berry curvature is also Guage invariant, because

$$\widetilde{\mathbf{A}} = \mathbf{A} + \nabla\beta,$$

For calculation purpose,

$$\Omega_n(\vec{R}) = i \sum_{m \neq n} \frac{\left\langle \Phi_n(\vec{R}) \middle| \nabla_{\vec{R}} \hat{\mathcal{H}} \middle| \Phi_m(\vec{R}) \right\rangle \times \left\langle \Phi_m(\vec{R}) \middle| \nabla_{\vec{R}} \hat{\mathcal{H}} \middle| \Phi_n(\vec{R}) \right\rangle}{(E_n(\vec{R}) - E_m(\vec{R}))^2}$$

TIME EVOLUTION OF A QUANTUM STATE

ADIABATIC APPROXIMATION Gradual change of $\widehat{\mathcal{H}}$ due to external parameters.

$$T_{external} \gg T_{internal} \equiv \frac{h}{E_{ab}} \longrightarrow \text{Time dependent perturbation}$$

ADIABATIC THEOREM If the n^{th} eigenstate of $\widehat{\mathcal{H}}_i$ adiabatically evolves to the n^{th} eigenstate of $\widehat{\mathcal{H}}_f$, then

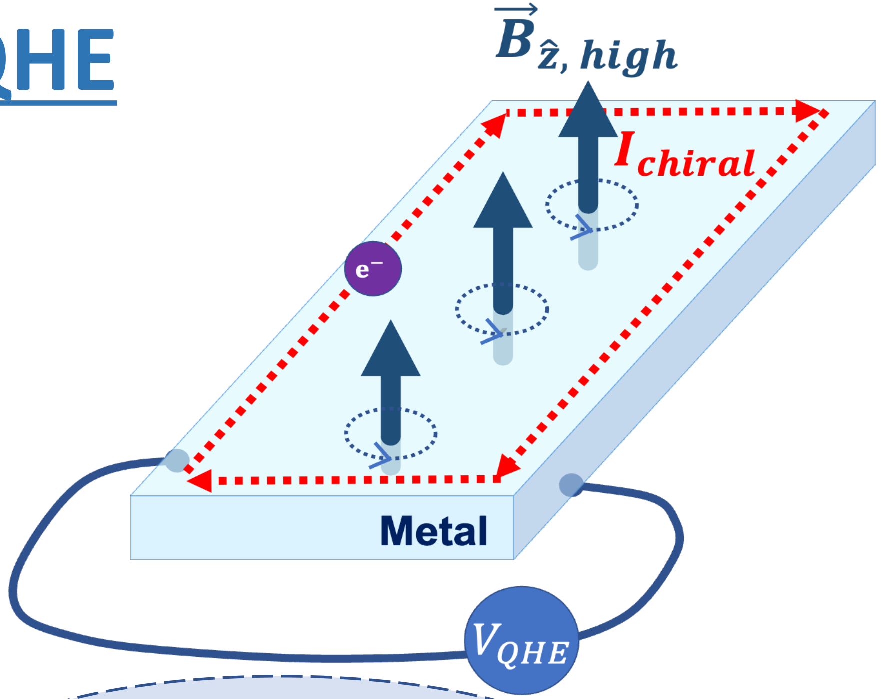
$$|\Psi_n(t)\rangle = \underbrace{e^{i\theta_n(t)}} * |\Psi_n(0)\rangle * e^{i\gamma_n(t)}$$

Time evolution operator , $\theta_n(t) = -\frac{2\pi}{h}\int_0^t E_n(t')\,dt'$

Berry Phase factor

J. J. Sakurai, Jim Napolitano, Modern Quantum Mechanics, Cambridge University Press, 2017

VELOCITY & BERRY CURVATURE IN QHE



In absence of any external charge, $$H = \frac{(\vec{P} - q\vec{A})^2}{2m^*}$$

So, the velocity is given by, $$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}} H(\mathbf{k})$$

It can be shown, $$\mathbf{v}_n(\mathbf{k}) = \langle n, \mathbf{k}(t)|\mathbf{v}|n, \mathbf{k}(t)\rangle$$
$$= \frac{1}{\hbar}\nabla_{\mathbf{k}} E[\mathbf{k}] + \frac{d\mathbf{k}(t)}{dt} \times \nabla_{\mathbf{k}} \times \langle n, \mathbf{k}|i\nabla_{\mathbf{k}}|n, \mathbf{k}\rangle$$

Berry curvature

By using,

$$\frac{d\mathbf{k}(\mathbf{t})}{dt} = \frac{e}{\hbar}\frac{\partial \mathbf{A}}{\partial t} = -\frac{e}{\hbar}\mathbf{E} \Rightarrow \mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}} E_n[\mathbf{k}] - \frac{e}{\hbar}\mathbf{E} \times \mathbf{\Omega}_n(\mathbf{k})$$

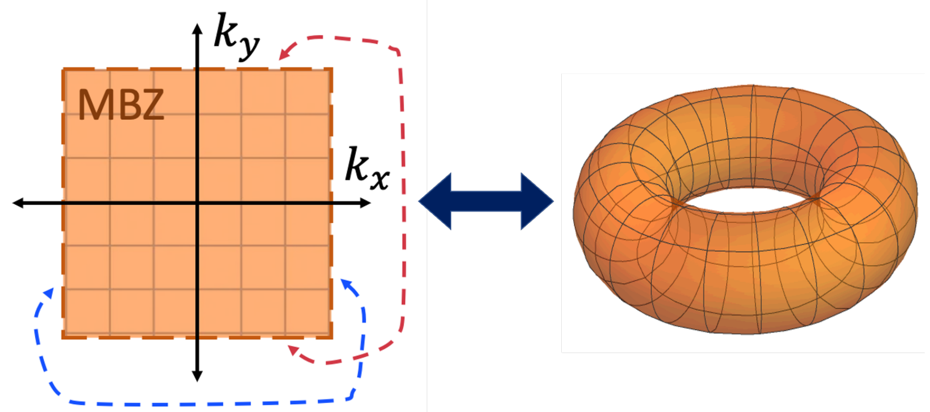
Anamolous velocity

HALL CONDUCTANCE & TKNN RELATION

The Hall conductivity is calculated using the Kubo formula,

$$\sigma_{xy} = \frac{e^2}{h}\frac{1}{2\pi i}\sum_{E\leq E_f}\iint_{MBZ} d^2k\left[\nabla_{\vec{k}} \times \vec{A}_{n,\vec{k}}\right]_z$$

$$\sigma_{xy} = \frac{e^2}{h}\sum_{n} C_n$$



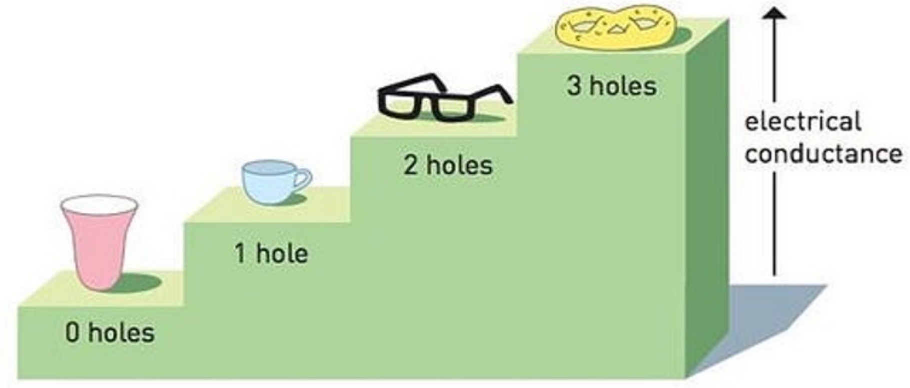
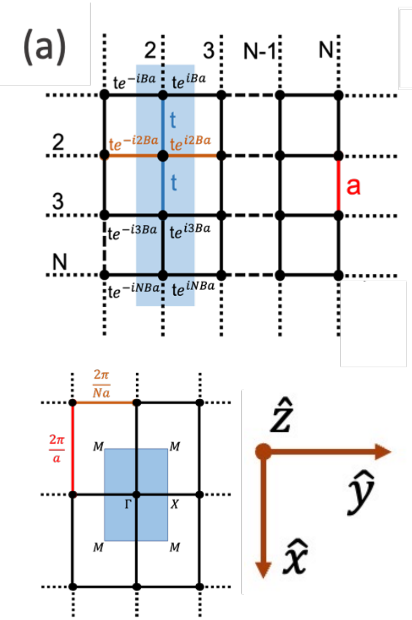
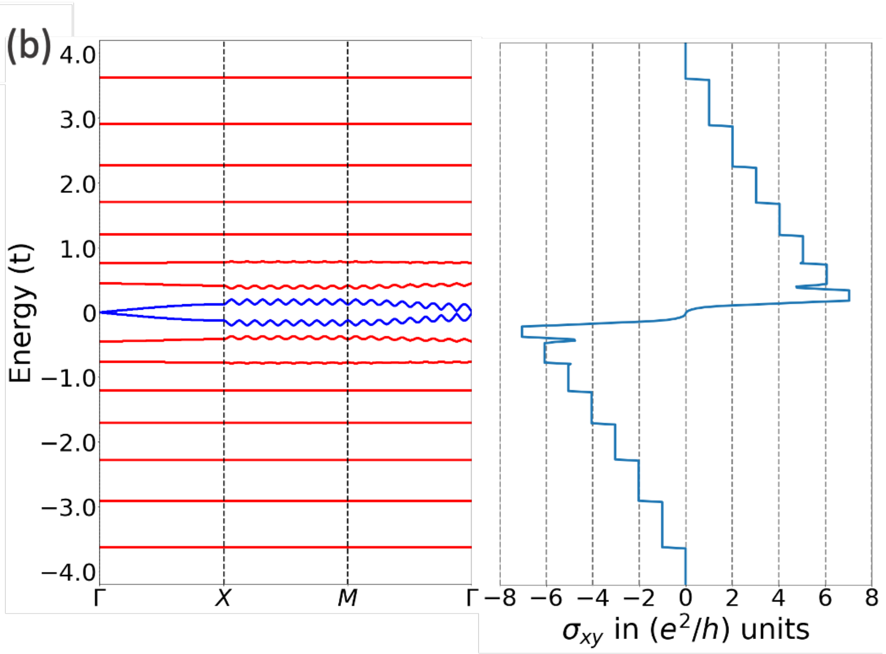


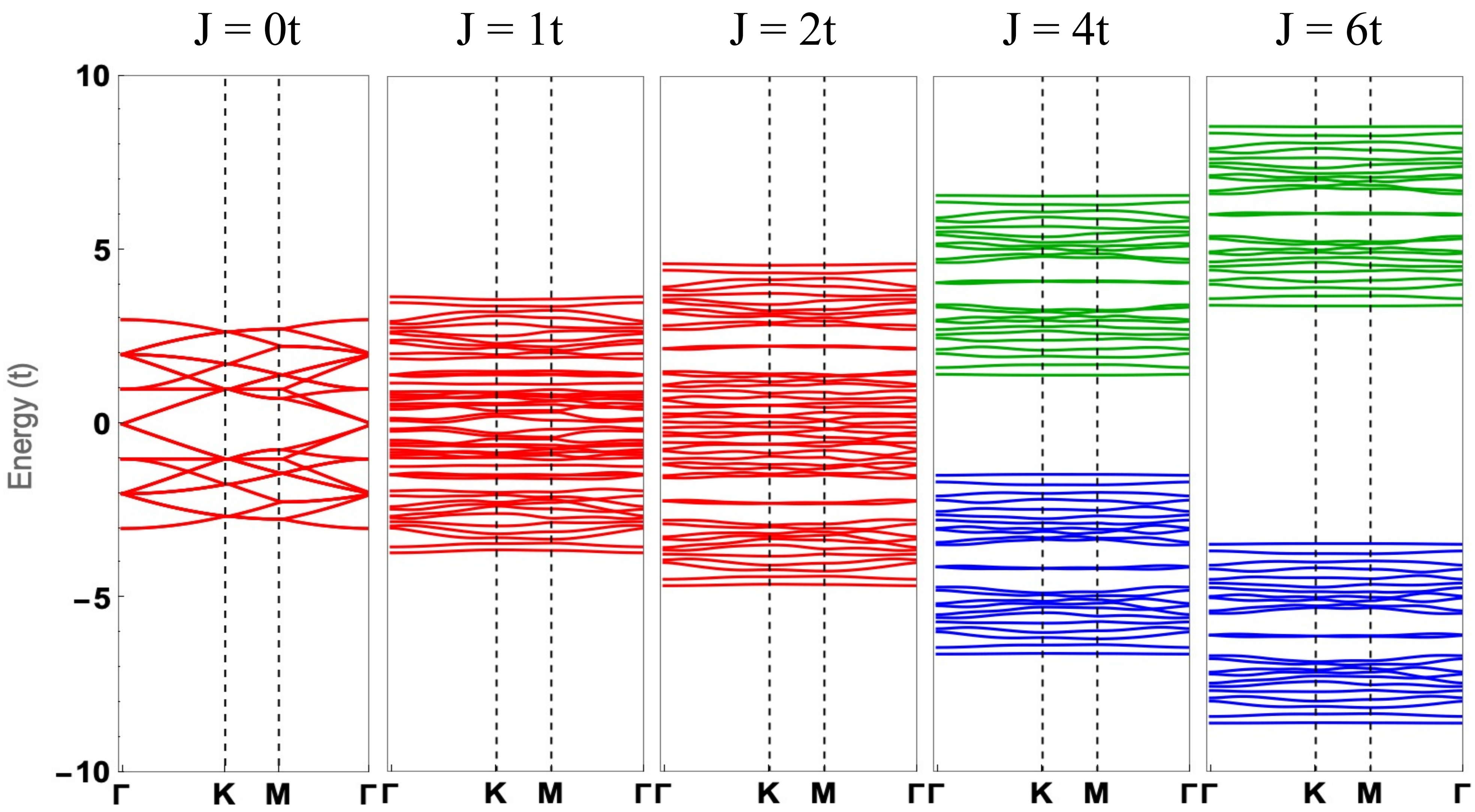
Illustration: ©Johan Jarnestad/The Royal Swedish Academy of Sciences

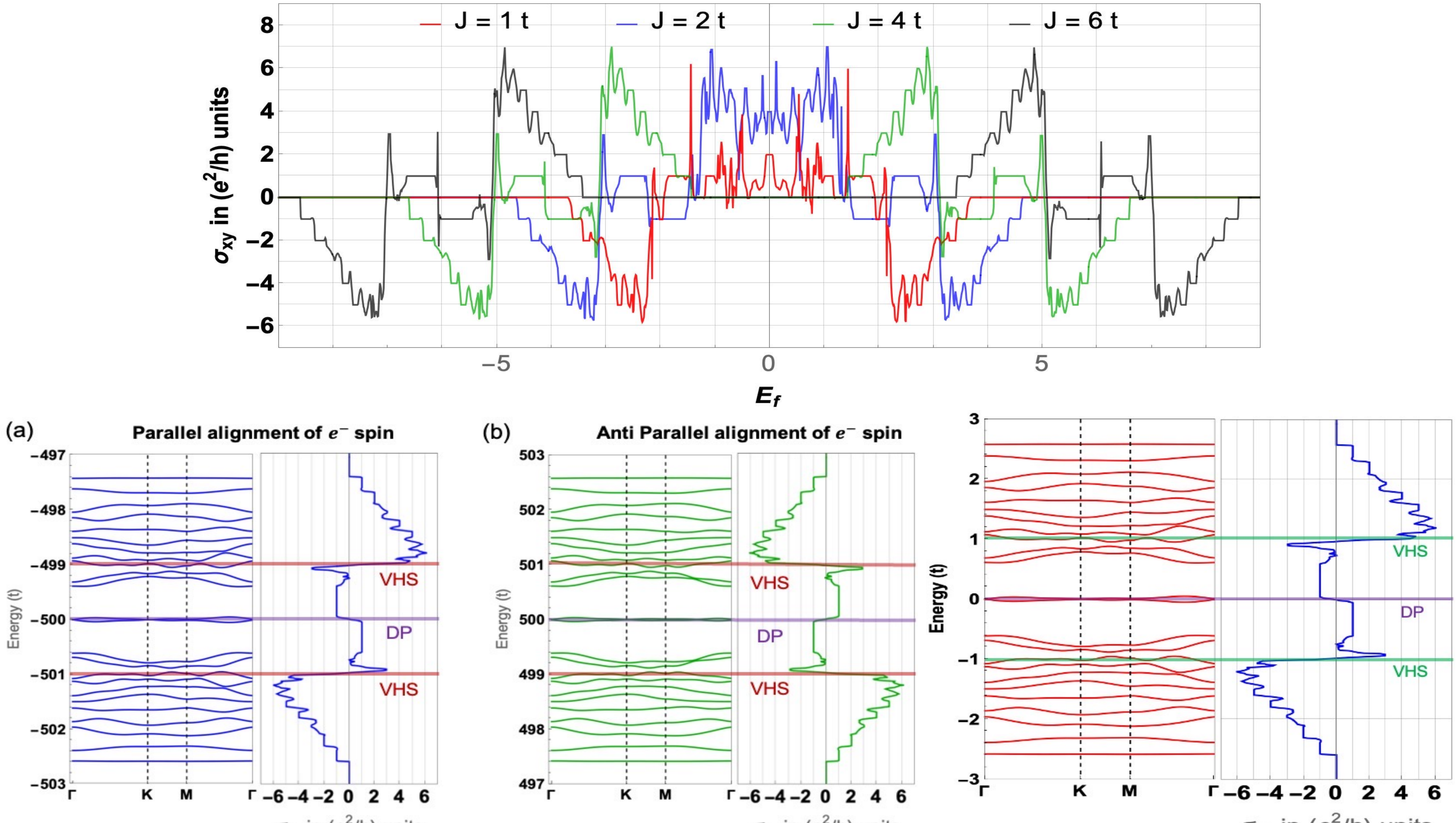




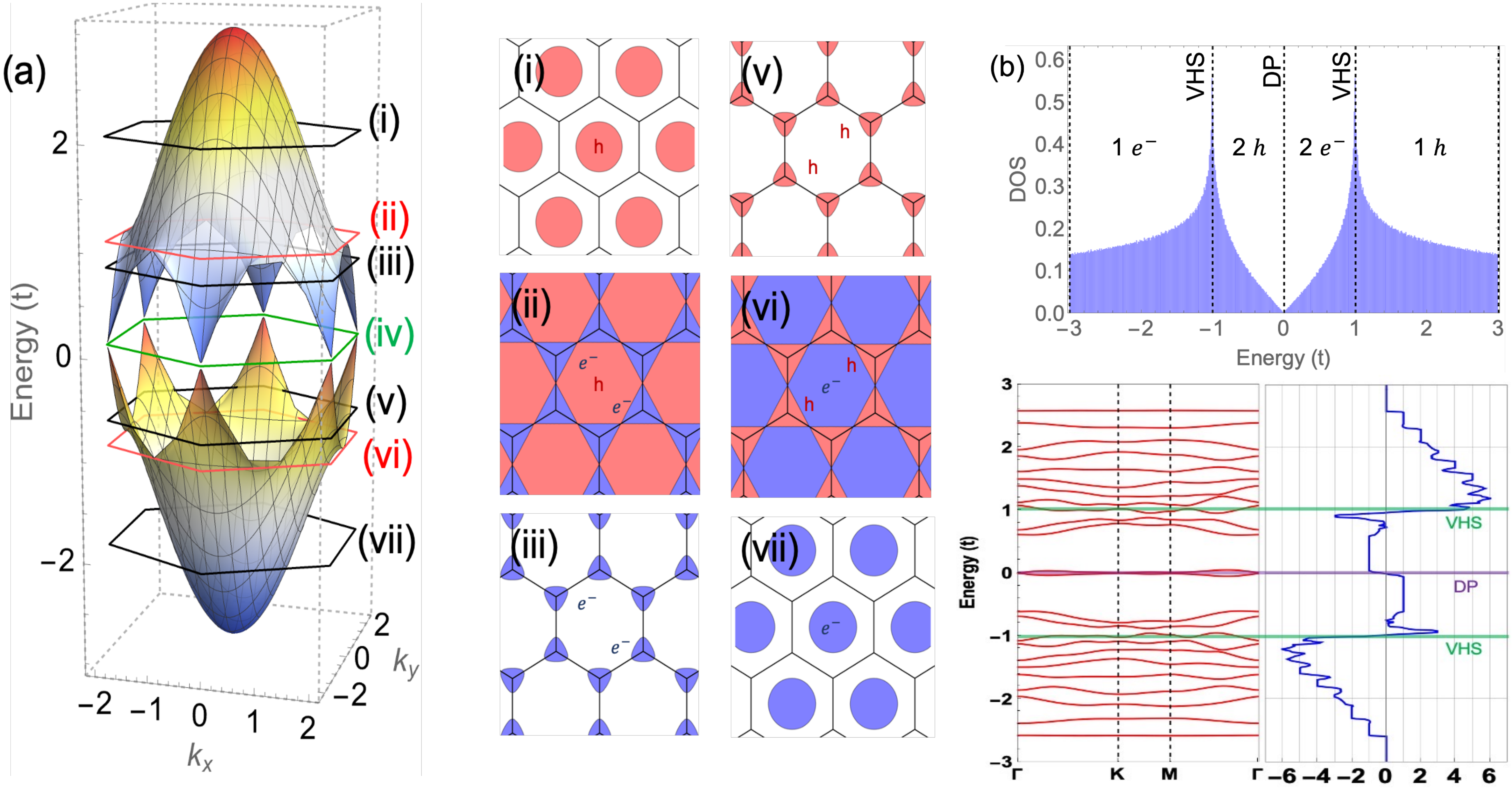
D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405

RESULTS FOR SkX IN A HONEYCOMB LATTICE





J = 1 t
J = 2 t
J = 4 t
J = 6 t
σ_{xy} in (e^2/h) units
E_f
(a)
Parallel alignment of e^- spin
(b)
Anti Parallel alignment of e^- spin
Energy (t)
VHS
DP
VHS
Γ
K
M
Γ
σ_{xy} in (e^2/h) units

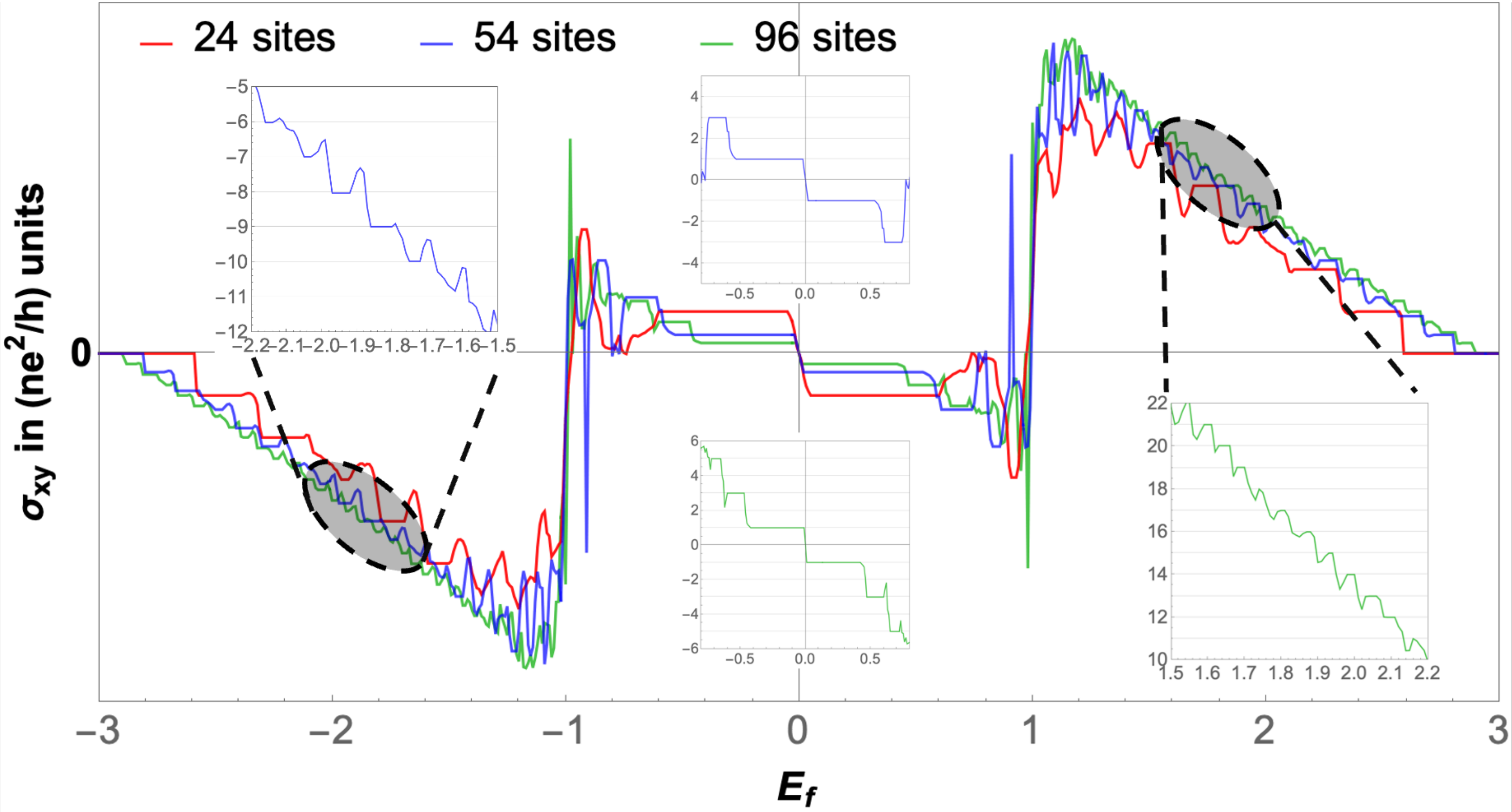


$$\zeta = n\,(j + 1/2)\zeta_o$$

$\zeta_0 = F/q$, F area of the Brillouin zone

SKYRMION SIZE EFFECTS

Börge Göbel *et al* 2017 *New J. Phys.* **19** 063042



EFFECTS OF RASHBA & DRESSELHAUS SOC

- The Rashba effect is a spin-orbit interaction that arises in materials with broken structural inversion symmetry.

$$\mathcal{H}_R = i\lambda_R \sum_{ij} c_i^\dagger \ (\sigma_x r_y - \sigma_y r_x) \ c_j$$

$$\mathcal{H}_R = i\lambda_R \sum_{ij} \langle \chi_i | r_y \sigma_x - r_x \sigma_y | \chi_j \rangle$$

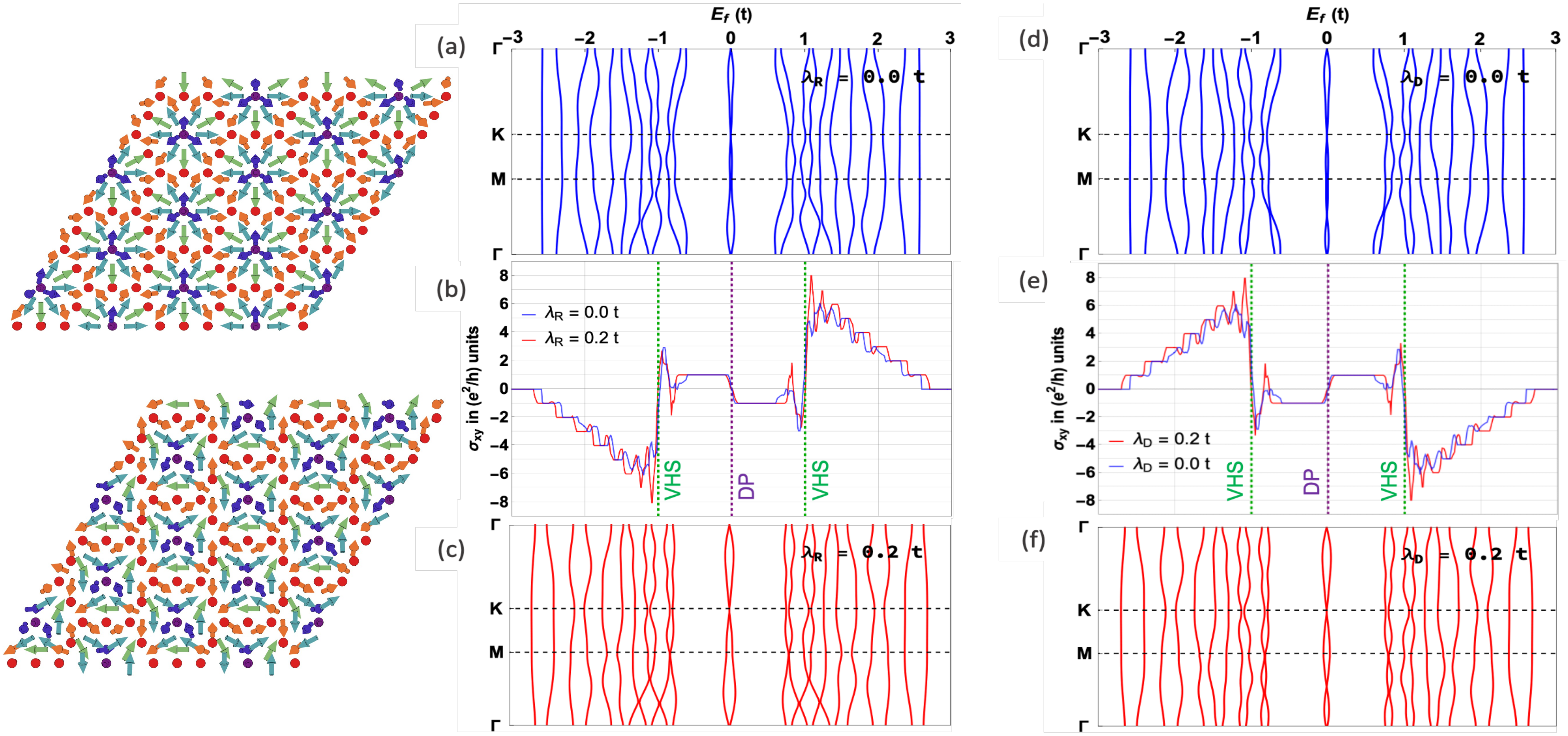
- The Dresselhaus is a spin-orbit interaction that arises in materials with broken bulk inversion symmetry.

$$\mathcal{H}_D = i\lambda_D \sum_{ij} c_i^\dagger \ (\sigma_x r_x - \sigma_y r_y) \ c_j$$

$$\mathcal{H}_D = i\lambda_D \sum_{ij} \langle \chi_i | r_x \sigma_x - r_y \sigma_y | \chi_j \rangle$$

EFFECTS OF RASHBA & DRESSELHAUS SOC

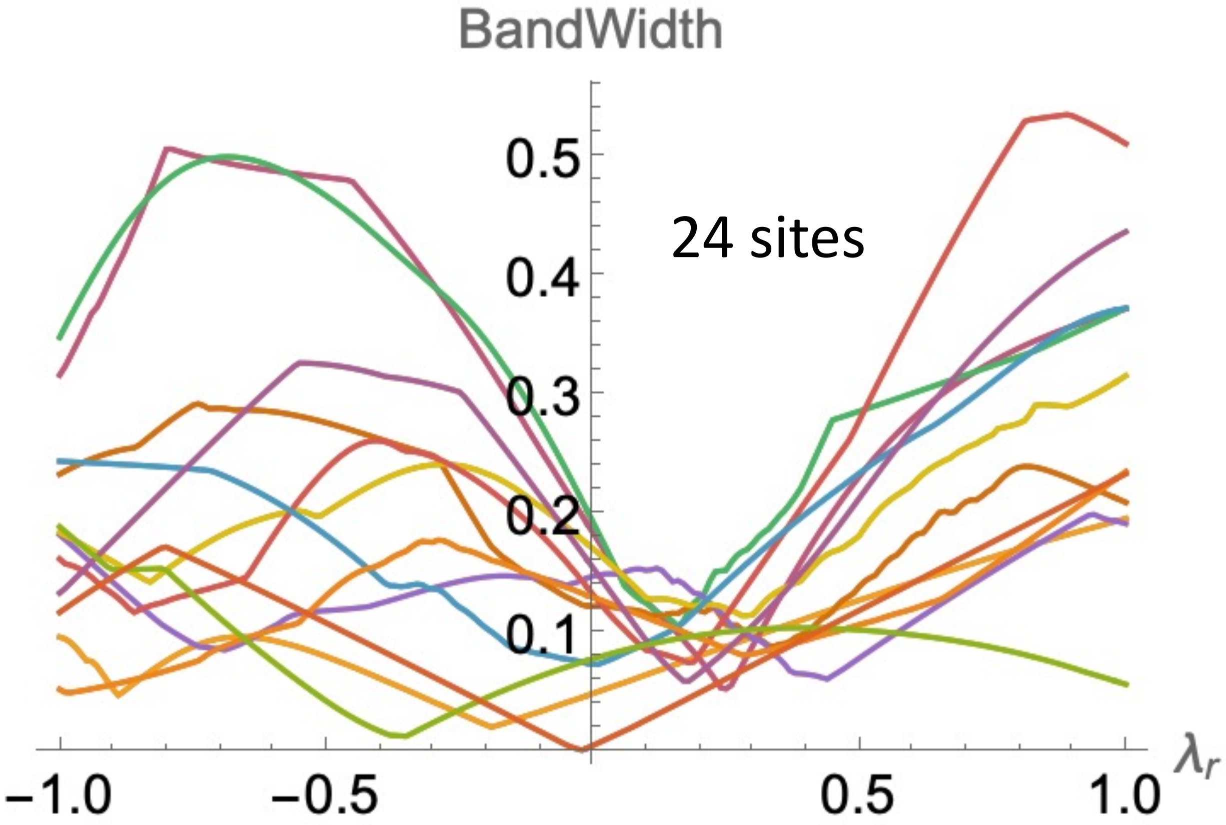
$$\phi_{sk} = N_{sk}\phi_o$$



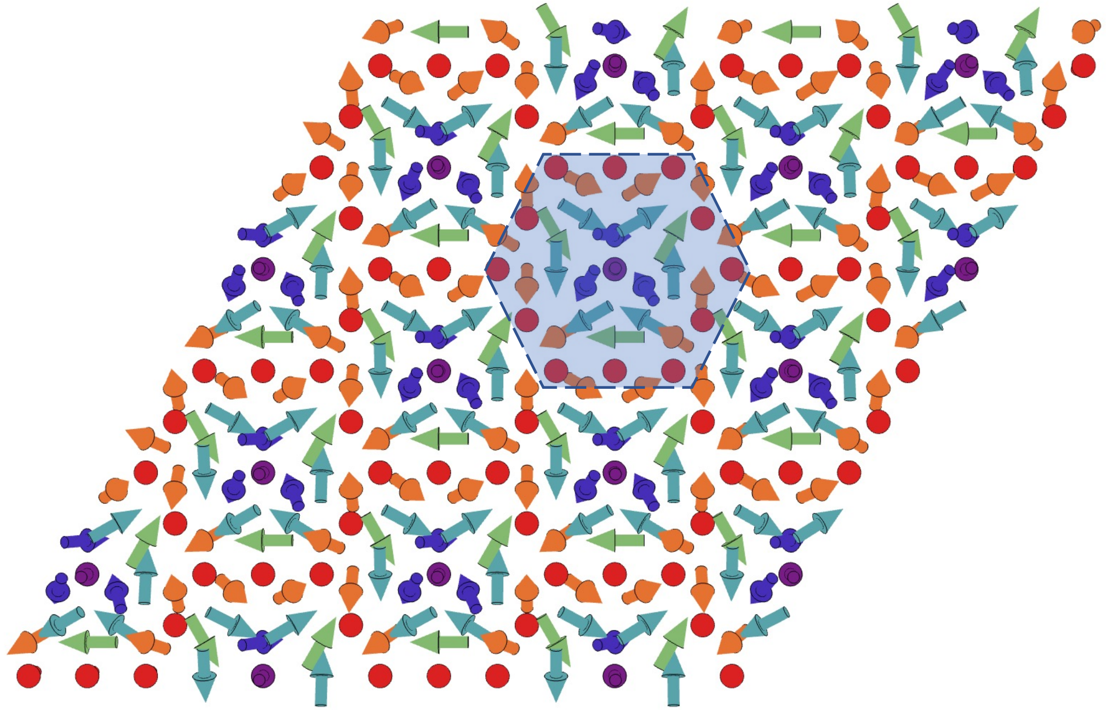
SUMMARY

1. QAHE due to skyrmion topology (QTHE) is numerically studied in the tight binding frame work. Code is developed in house.
2. In numerical analysis the Rashba effect on Neel skyrmion and Dresselhaus effect on Bloch antiskyrmion are consistent with the literature for a snigle skyrmion continuum model.

THANK YOU !



BandWidth
24 sites
0.5
0.4
0.3
0.2
0.1
−1.0
−0.5
0.5
1.0
λ_r



GUAGE FREEDOM & BERRY POTENTIAL

$$\boldsymbol{\varphi} = \oint \langle \boldsymbol{u_\lambda} | \boldsymbol{i}\overrightarrow{\nabla_\lambda} | \boldsymbol{u_\lambda} \rangle \,.\, \boldsymbol{d\vec{\lambda}} = \oint \vec{A}\,(\vec{\lambda}).\,\boldsymbol{d\vec{\lambda}}$$

Make a general Guage Transformation,

$$|\tilde{u}_j\rangle = e^{-i\beta_j}\,|u_j\rangle$$

$$\widetilde{A}(\lambda) = \langle \tilde{u}_\lambda | i\partial_\lambda | \tilde{u}_\lambda \rangle$$

$$= \langle u_\lambda | e^{i\beta(\lambda)}\, i\partial_\lambda\, e^{-i\beta(\lambda)} | u_\lambda \rangle$$

$$\widetilde{A}(\lambda) = A(\lambda) + \beta'(\lambda)$$

Since a general Guage Transformation,

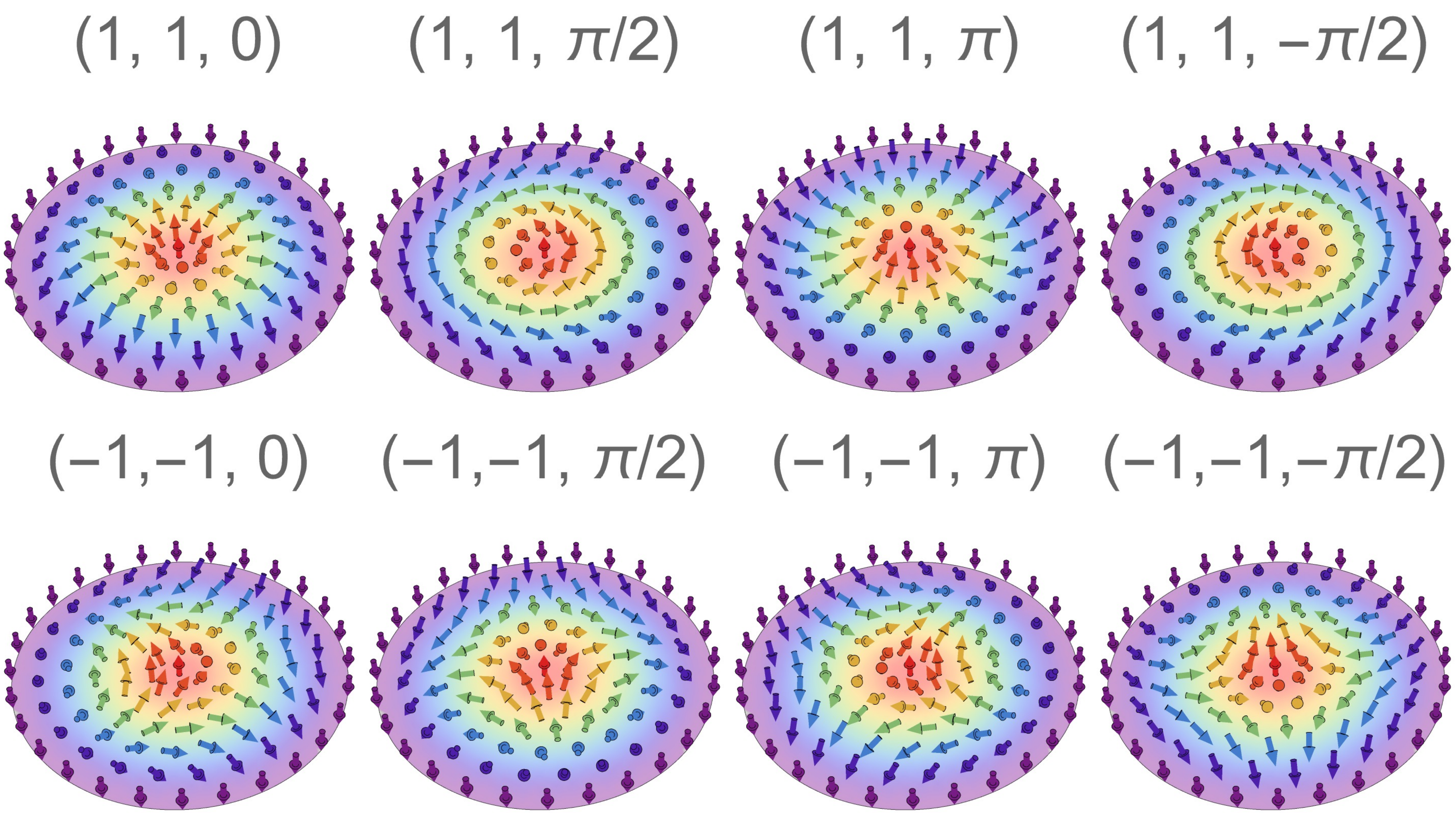
$$|\tilde{u}_{\lambda=1}\rangle = |\tilde{u}_{\lambda=0}\rangle$$

$$\Longrightarrow \quad \beta_{\lambda=1} = \beta_{\lambda=0} + 2\pi m$$

Change in Berry phase is,

$$\int_0^1 \beta'(\lambda)\, d\lambda = \beta_{\lambda=1} - \beta_{\lambda=0} = 2\pi m$$

$\tilde{\phi} = \phi + 2\pi m$ $\Longrightarrow$ Guage invariance !



(1, 1, 0)
(1, 1, π/2)
(1, 1, π)
(1, 1, −π/2)
(−1,−1, 0)
(−1,−1, π/2)
(−1,−1, π)
(−1,−1,−π/2)