

- ★ *Berry phase, extension of KSV formula & Chern number*
- ★ *Berry connection ?*
- ★ *TKNN number & Hall conductance*
- ★ *One body to many body*
- ★ *extension of the KSV formula*
- ★ *Numerical examples: graphene*

Y. Hatsugai
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Berry connection, Chern numbers ?

Eigen vector? $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = E \begin{pmatrix} a \\ b \end{pmatrix} \quad E = \pm 1$

$E =$

If a

Gauge Freedom
M.V. Berry, '84

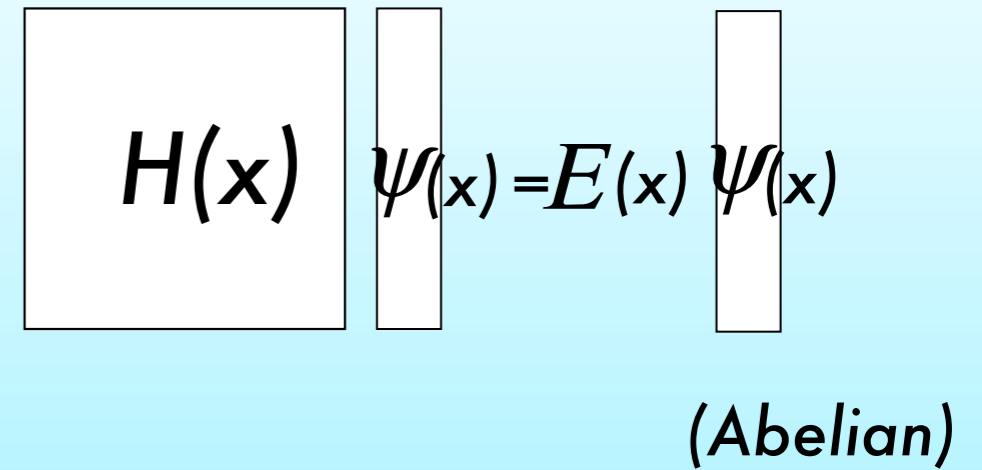
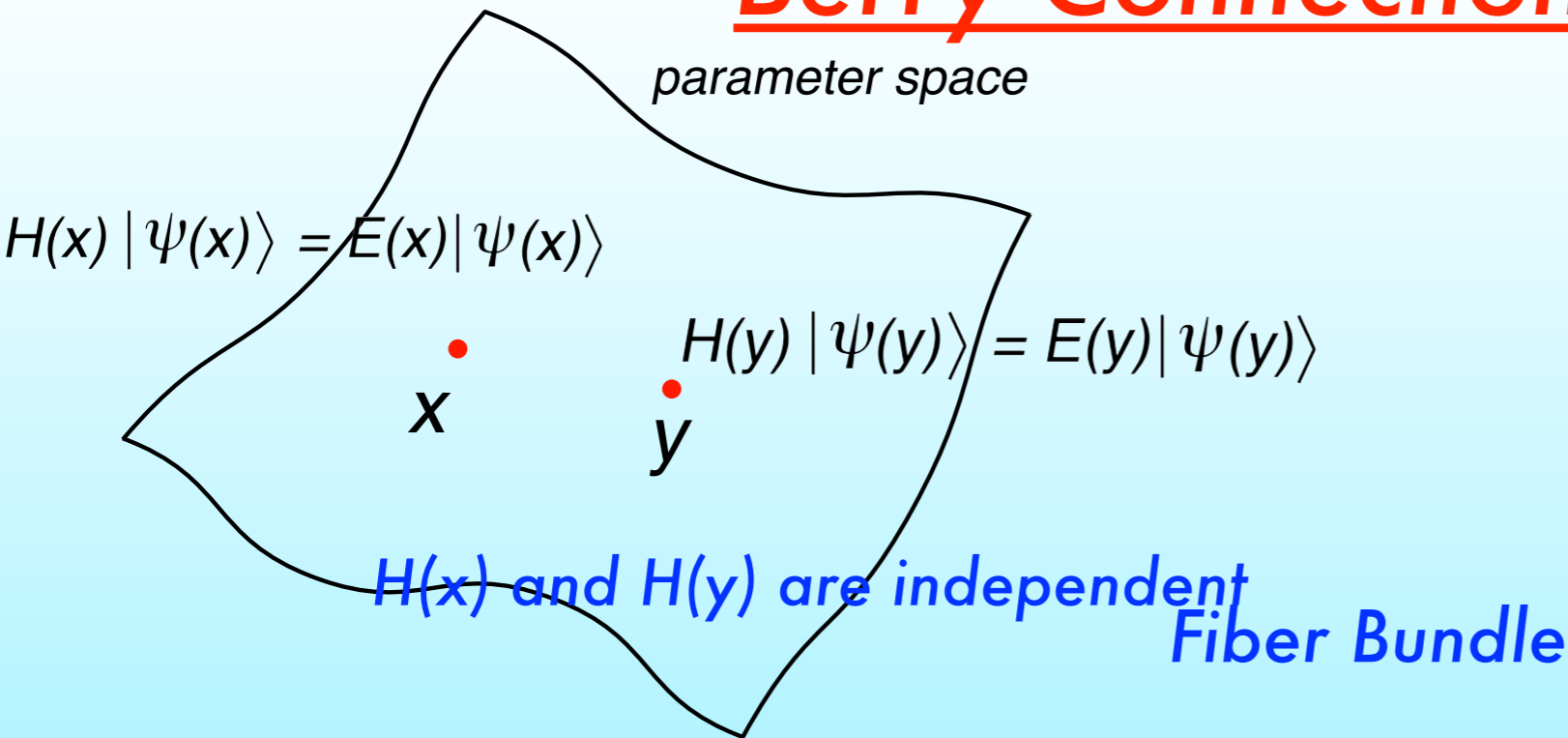
$a = 1$!!

Can we do this? $\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$? $a = 0$!!!!
choice is singular

Is it all ? No! $\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ -1 \end{pmatrix}, \begin{pmatrix} 0 \\ i \end{pmatrix}, \begin{pmatrix} 0 \\ e^{i\theta} \end{pmatrix}$
phase is arbitrary

Berry Connection

Eigenvectors (space)
with Parameters



Information between nearby states

Berry connection : $A_\psi = \langle \psi | d\psi \rangle = \langle \psi | \frac{d}{dx} \psi \rangle dx.$

Gauge Transformation

$$|\psi(x)\rangle = |\psi'(x)\rangle e^{i\Omega(x)}$$

$$A_\psi = A'_\psi + id\Omega = A'_\psi + i \frac{d\Omega}{dx} dx$$

Geometrical quantities

gauge potential

$$i\gamma_C(A_\psi) = \int_C A_\psi \quad : \text{Berry phase}$$

Spectral Flow and Berry's Connection

★ Spectral Flow

★ Hamiltonian depends on Some parameters $H(x)$

★ Eigenstate Energies as a Function of Some Parameters $E_n(x)$

$$H(x)|n(x)\rangle = E_n(x)|n(x)\rangle$$

★ Berry's Connection

$$\mathcal{A} = \langle n|d|n\rangle$$

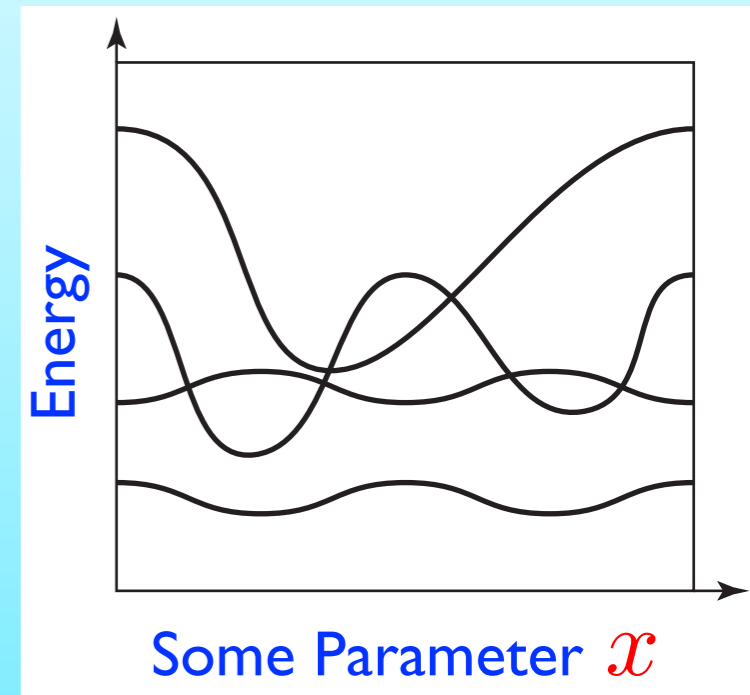
$$\vec{A} = \langle n|\vec{\nabla}|n\rangle$$

★ Phase Ambiguity \longrightarrow Gauge Freedom

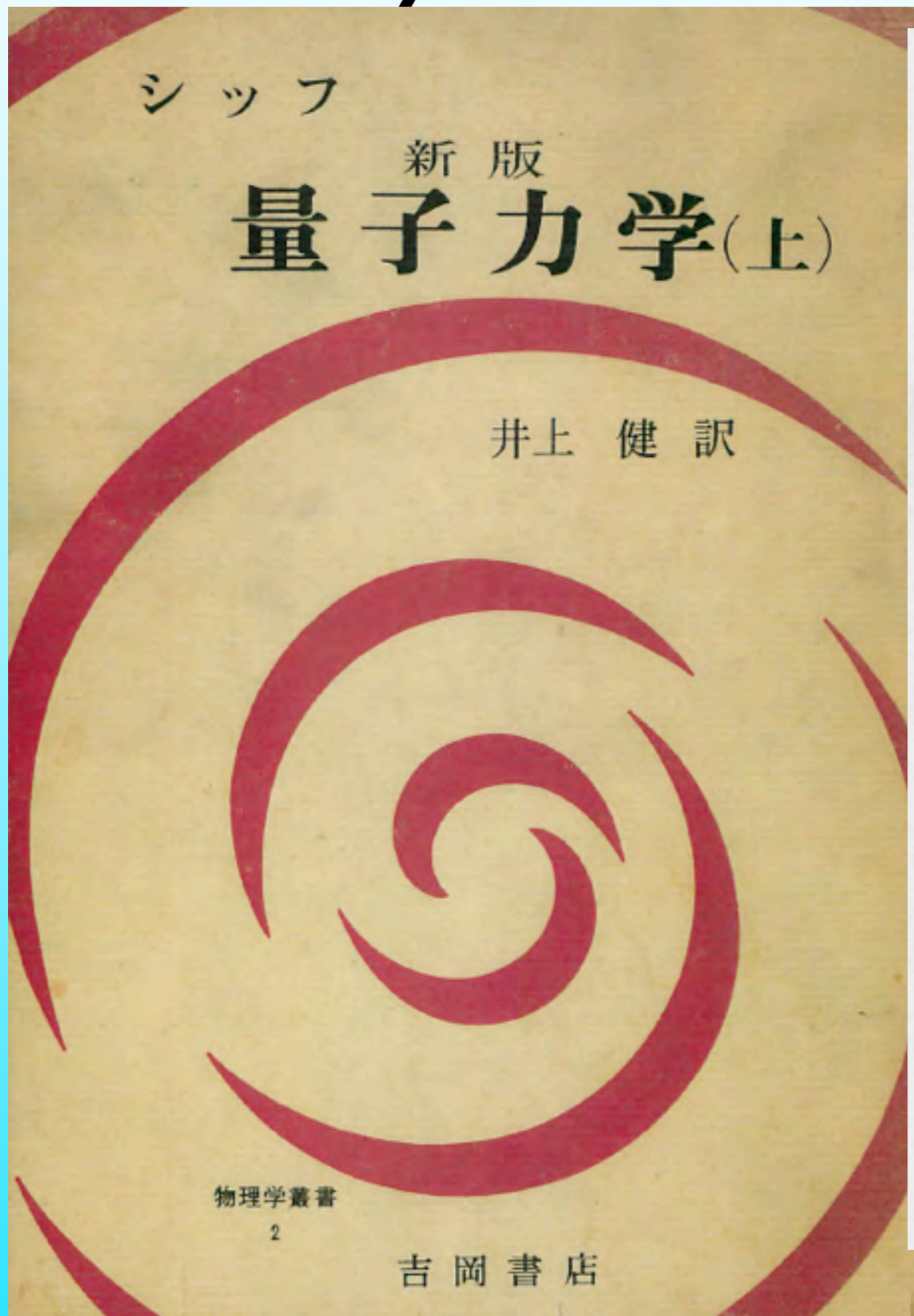
$$|n(x)\rangle' = e^{i\theta(x)}|n(x)\rangle$$

$$\mathcal{A}' = \mathcal{A} + id\theta$$

$$\vec{A}' = \vec{A} + i\vec{\nabla}\theta$$



Berry connection in a textbook



336

第V章 束縛状態に対する近似法

$\langle k|n \rangle$ に対する表式は、(35.21) を時間について微分して求めることができる；すなわち

$$\frac{\partial H}{\partial t} u_n + H \frac{\partial u_n}{\partial t} = \frac{\partial E_n}{\partial t} u_n + E_n \frac{\partial u_n}{\partial t}.$$

ここで $k \neq n$ として u_k^* を左からかけて全空間にわたって積分し、(23.21) と (35.21) を使うと次の関係が得られる。

$$\langle k | \frac{\partial H}{\partial t} | n \rangle = (E_n - E_k) \langle k | n \rangle \quad \text{ただし } k \neq n. \quad (35.25)$$

35-11 位相の選び方

さらに $\langle n|n \rangle$ に対する表式が必要である。方程式 $\langle n|n \rangle = 1$ を時間について微分すれば次の関係が与えられる。

$$\langle n|n \rangle + \langle n|n \rangle = 0$$

これらの二つの項は互いに共軛な複素量になっているから、この関係によってそれぞれは純虚量になり、したがって $\alpha(t)$ を実数として $\langle n|n \rangle = i\alpha(t)$ と書くことができる。ここで u_n の位相を大きさ $\gamma(t)$ だけ変化させてみる。固有関数の位相は各瞬間で任意である以上、このような変更は許されていることである。この新しい固有関数 $u_n' = u_n e^{i\gamma(t)}$ に対しては

$$\langle n'|n' \rangle = \langle n|n \rangle + i\dot{\gamma} = i(\alpha + \dot{\gamma})$$

となる。したがってこの新しい固有関数の位相に対して $\gamma(t) = -\int_0^t \alpha(t') dt'$ という選び方をしておくと、 $\langle n'|n' \rangle = 0$ となる。以下ではすべての位相はこのようなやり方で選ばれてきているものと仮定して、'は省略することにする。

A=0 OK!

ONLY LOCALLY!

Topological meaning of the Hall Conductance

★ **TKNN formula: σ_{xy} as a topological invariant**

Kubo formula

$$\sigma_{xy} = \frac{e^2}{h} \sum_{\ell: \epsilon_{\ell}(k) < E_F} C_{\ell}$$

Thouless-Kohmoto-Nightingale-den Nijs '82

Sum over the bands below E_F

$$C_{\ell} = \frac{1}{2\pi i} \int_{T^2: \text{BZ}} F_{\ell}$$

:First Chern number of the ℓ -th Band

intrinsically integer

unless the energy gap collapses

$$\forall k, \epsilon_{\ell}(k) \neq \epsilon_{\ell \pm 1}(k)$$

regularity of the Berry connection

$$F_{\ell} = dA_{\ell} = \langle d\psi_{\ell} | d\psi_{\ell} \rangle$$

$$A_{\ell} = \langle \psi_{\ell} | d\psi_{\ell} \rangle$$

$$H(k) |\psi_{\ell}(k)\rangle = \epsilon(k) |\psi_{\ell}(k)\rangle$$

$$k \in T_{\text{BZ}}^2 = \{k = (k_x, k_y) \mid 0 \leq k_x, k_y \leq 2\pi\}$$

$$d = dk_{\mu} \frac{\partial}{\partial k_{\mu}}$$

One-body to Many-body

Berry phases,...

one particle problem

$$H(\phi)|\psi_j(\phi)\rangle = \epsilon_j(\phi)|\psi_j(\phi)\rangle$$

Twisted boundary conditions

$$\phi = (\phi_x, \phi_y)$$

$$\sigma_{xy} = \frac{e^2}{h} \frac{1}{2\pi i} \int_{T^2} d\mathcal{A} = \frac{e^2}{h} \frac{1}{2\pi i} \int_{T^2} \text{Tr}_M dA_{FS}$$

Niu-Thouless-Wu formula

TKNN formula

$$|G\rangle = \prod_{\ell=1}^M (\mathbf{c}^\dagger \psi_\ell) |0\rangle$$

M particle state: filled Dirac sea

$$\mathcal{A} = \langle G | dG \rangle = \text{Tr}_M A_{FS}$$

Many-body from one-body

$\Psi = (|\psi_1\rangle, \dots, |\psi_M\rangle)$ Collect M states below the Fermi level

$$A_{FS} \equiv \Psi^\dagger d\Psi = \begin{pmatrix} \langle \psi_1^\dagger | d\psi_1 \rangle & \cdots & \langle \psi_1^\dagger | d\psi_M \rangle \\ \vdots & \ddots & \vdots \\ \langle \psi_M^\dagger | d\psi_1 \rangle & \cdots & \langle \psi_M^\dagger | d\psi_M \rangle \end{pmatrix}$$

Matrix vector potential of the Fermi (Dirac) Sea

Non Abelian extension for the Chern numbers

YH 2004

Topological meaning of the Hall Conductance

When E_F is in the j -th gap Two topological quantities

★ $\sigma_{xy}^{\text{bulk}} = \frac{e^2}{h} \sum_{\ell: \epsilon_{\ell}(k) < E_F} C_{\ell}$ Sum of the First Chern numbers below E_F
 Thouless-Kohmoto-Nightingale-den Nijs '82
 Phys. Rev. Lett. 49, 405–408 (1982)

★ $\sigma_{xy}^{\text{edge}} = \frac{e^2}{h} I(\alpha_j, C^j)$ Winding number of the edge state
 in the complex energy surface Hatsugai '93a
 Phys. Rev. B 48, 11851–11862 (1993)

Bulk — Edge Correspondence Hatsugai '93b

$$\sigma_{xy}^{\text{bulk}} = \sigma_{xy}^{\text{edge}}$$

Phys. Rev. Lett. 71, 3697–3700 (1993)

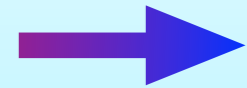
Chern Numbers:

Total Flux of Berry's Connection

★ Fictitious Flux Density

$$\mathcal{B} = d\mathcal{A}$$

$$\vec{B} = \vec{\nabla} \times \vec{A} = \text{rot } \vec{A}$$



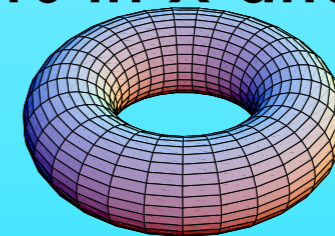
★ Total Flux over the Parameter Space is the Chern Number C

$$\begin{aligned} C &= \frac{1}{2\pi i} \int_S \mathcal{B} = \frac{1}{2\pi i} \int_S d\mathcal{A} \\ &= \frac{1}{2\pi i} \int_S d\vec{S} \cdot \vec{B} \end{aligned}$$

★ What is the SURFACE S ?

For the QHE, specifying two twisting parameters in x and y directions

$$S = \{(\phi_x, \phi_y) \mid \phi_{x,y} \in [0, 2\pi]\} = T^2$$



Torus
(No Boundary)

★ This is Always Integer due to generic Topological Reasons

Chen Number for Superconductors

PRB65, 212510-1-4(2002), B70, 0545-2 (2004)

★ BCS Hamiltonian (2×2) and Parametrization

$$h(\mathbf{k}) = \begin{pmatrix} \epsilon(\mathbf{k}) & \Delta(\mathbf{k}) \\ \Delta^*(\mathbf{k}) & -\epsilon(\mathbf{k}) \end{pmatrix} = \boldsymbol{\sigma} \cdot \mathbf{R}(\mathbf{k}) : \mathbf{k} \rightarrow \mathbf{R} = (R_x, R_y, R_z)$$

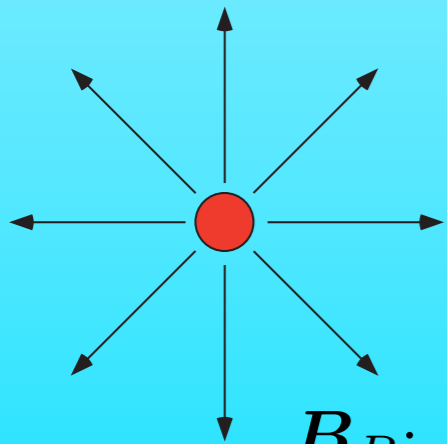
$$h|R\rangle = E_{\pm}|R\rangle, \quad E_{\pm} = \pm|\mathbf{R}|, \quad |R\rangle = \begin{pmatrix} -\sin\frac{\theta}{2} \\ e^{i\phi}\cos\frac{\theta}{2} \end{pmatrix} \quad (\text{Berry})$$

★ Chern Number and Dirac Monopole

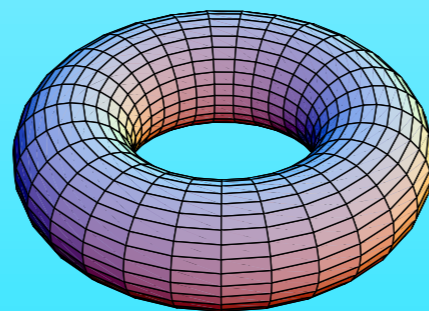
$$C = \frac{1}{2\pi i} \int_{BZ} d\mathbf{S}_k \cdot \mathbf{B}_k = \frac{1}{2\pi i} \int_{BZ} dk_x dk_y \left(\langle \partial_x k | \partial_y k \rangle - \langle \partial_y k | \partial_x k \rangle \right) : \sigma_{xy} \quad (\text{TKNN})$$

$$= \frac{1}{2\pi i} \int_{R(BZ)} d\mathbf{S}_R \cdot \mathbf{B}_R, \quad \mathbf{B}_R = \text{rot}_R \mathbf{A}_R, \quad \mathbf{A}_R = -\frac{i}{2} \frac{\mathbf{R}}{R^3}, \quad \mathbf{A}_R = \langle R | \nabla R \rangle$$

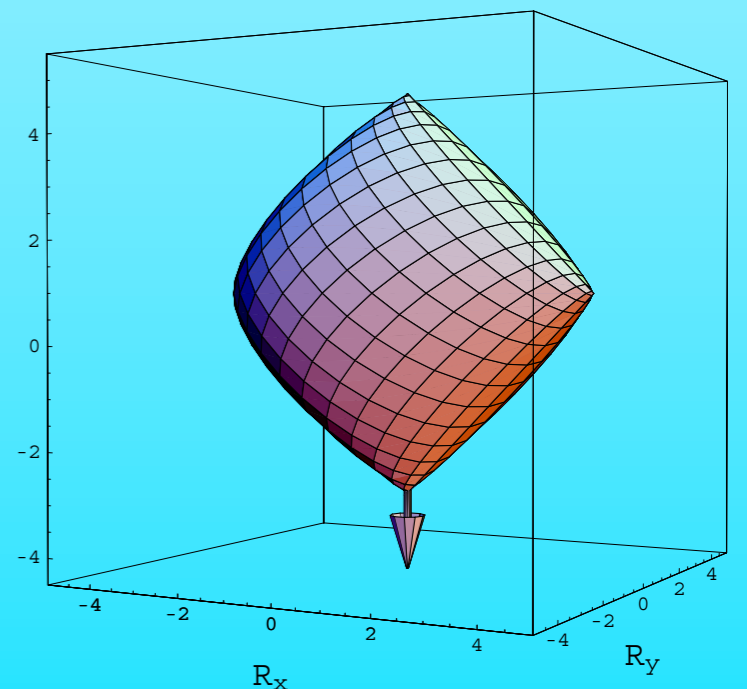
$$= - \int_{V, \partial V=R(BZ)} dV \delta(\mathbf{r}) = \boxed{-N_{\text{covering}}}$$



\mathbf{B}_R : Monopole at the Origin



Brillouin Zone



Chern Number and Berry's Connection

★ Berrys' Connection (ex. Quantum Hall Effect)

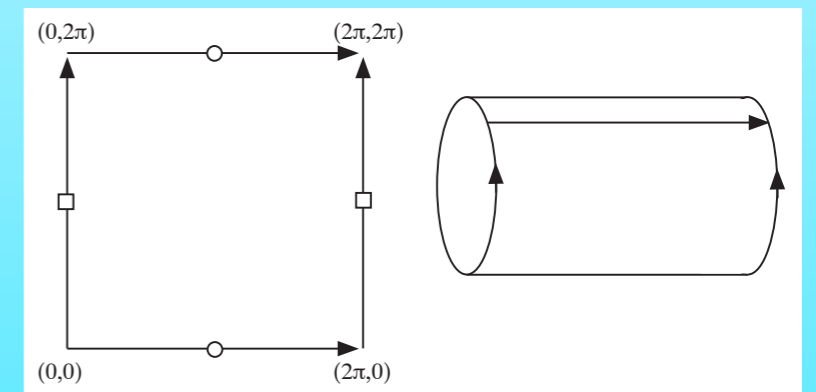
$$A = \langle n | dn \rangle = A_\mu dk_\mu = \langle n | \partial_\mu n \rangle dk_\mu \quad \mu = 1, 2, \vec{k} = (k_1, k_2)$$

$$H(k) |n(k)\rangle = E(k) |n(k)\rangle \quad \vec{k} = (k_1, k_2) \in \text{2D Brillouin Zone}$$

$$F = dA = \langle dn | dn \rangle = (\partial_1 A_2 - \partial_2 A_1) dk_1 \wedge dk_2 = F_{12} d^2 k$$

★ Chern Number as a Total Flux over the 2D BZ

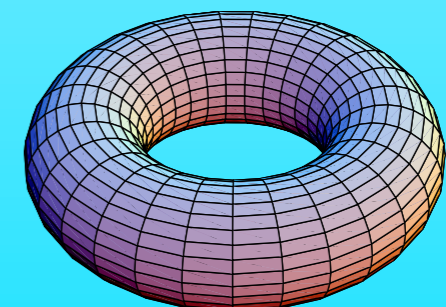
$$C = \frac{1}{2\pi i} \int_{T^2} F = \frac{1}{2\pi i} \int_{T^2} d^2 k F_{12}$$



2D Brillouin zone is a torus

$$\sigma_{xy} = \frac{e^2}{h} \sum_{E(k) < E_F} C$$

Hall Conductance




Berry's Connection and Gauge Freedom

★ Phase of different k points is independent!

Gauge Freedom

$$H(k)|n(k)\rangle = E(k)|n(k)\rangle$$


$$H(k)(|n(k)\rangle e^{i\theta(k)}) = E(k)(|n(k)\rangle e^{i\theta(k)})$$

$$|n\rangle \rightarrow |n\rangle' = |n\rangle \omega, \quad \omega = e^{i\theta}, \theta \in \mathbb{R} \quad : k \text{ dependent!}$$

$$A \rightarrow A' = \langle n|d|n\rangle' = A + \omega^\dagger d\omega = A + id\theta$$

$$F \rightarrow F' = dA' = F$$

★ **Gauge Fixing** $|\phi\rangle$: Arbitrary State

$$|n^\phi\rangle = P|\phi\rangle/N_\phi, \quad \text{Only if } N_\phi \neq 0$$

$$P = |n\rangle\langle n| \quad : \text{Projection to the state } |n\rangle$$

$$N_\phi = |\langle\phi|n\rangle| \quad : \text{Normalization for } \langle n^\phi|n^\phi\rangle = 1$$

Gauge Dependent Topological Expression

★ The Chern Number is always Zero ??

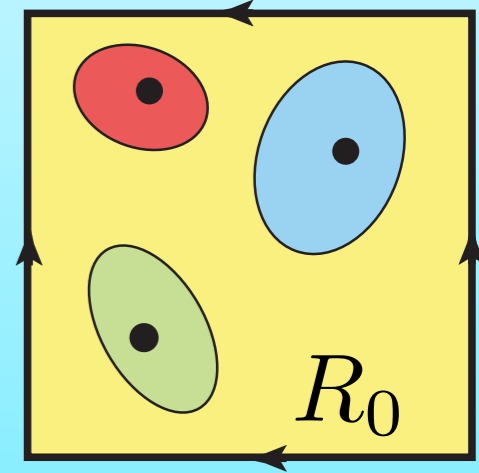
$$C = \frac{1}{2\pi i} \int_{T^2} dA \stackrel{\text{Stokes Theorem}}{=} \frac{1}{2\pi i} \int_{\partial T^2} A \stackrel{\text{No Boundary}}{=} 0 \quad ??$$

Wrong!
 $N_\phi = |\langle \phi | n \rangle|$
can be zero

★ Patch work on BZ to avoid singularities

Use Several (local) $|\phi\rangle$

$$N_\phi(k) = 0$$



$$C = \frac{1}{2\pi} \oint_{\partial R_0} d\Omega = N_\Omega(R_0)$$

$$|n\rangle_R = |n\rangle_0 \omega_{0R}$$

$$A_R = \omega_{0R}^{-1} A_0 \omega_{0R} + \omega_{0R}^\dagger d\omega_{0R}$$

$$\Omega = \text{Arg} \langle \phi' | P | \phi \rangle$$

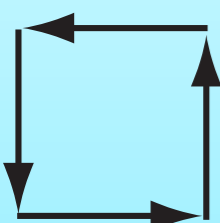
$$= \text{Arg} \frac{\langle n | \phi \rangle}{\langle n | \phi' \rangle}$$

Intrinsically Integer Topological !

Gauge Dependent !

Chern

★ Link
 $U_\mu(k_\ell)$: U

$\tilde{F}_{12}(k_\ell)$
 : \tilde{F}

第20回 (2015年) 論文賞授賞論文

20th Outstanding Paper Award of the Physical Society of Japan

in Zone

Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances

J. Phys. Soc. Jpn. 74, pp. 1674-1677 (2005)

Takahiro Fukui, Yasuhiro Hatsugai, and Hiroshi Suzuki

固体中の電子のトポロジカル状態は、電子物性の新しい理解のあり方として、あるいは将来的な応用にもつながりうる新物性発現の指針として注目され、その研究は物性物理学の理論研究における大きな潮流となりつつある。特に最近では具体的な物質を想定したモデル計算や第一原理に基づく電子状態計算を使って、トポロジカル状態を実現する新物質の提案まで行われるようになってきた。

これらの計算でトポロジカル状態かどうかを理論的に判定するには、逆格子空間での積分量で表されるトポロジカル数 (Chern Number) の計算が不可欠であるが、従来用いられていた離散化による数値積分手法は、ゲージ不変性に関する基本的困難に加え、積分に用いる離散点の数に対する収束性が極めて悪いこと、すなわち多くの離散点の情報が必要であることが深刻な問題となっていた。

これに対して本論文は、格子ゲージ理論の手法を応用して、離散点の情報を用いてゲ

2 皆さんもジャーナルに論文を投稿しましょう

り、トポロジカル状態の研究に本質的な寄与をする手法提案である。本論文は発表後10年が経過しているが、近年急激に認知度が上がり、当研究分野で世界中の研究者によって幅広く活用されるようになった。アイデアの斬新さにおいても、トポロジカル絶縁体・超伝導体の分野への貢献度の高さにおいても秀でており、日本物理学会論文賞に相応しい卓越した論文である。



★ Chern

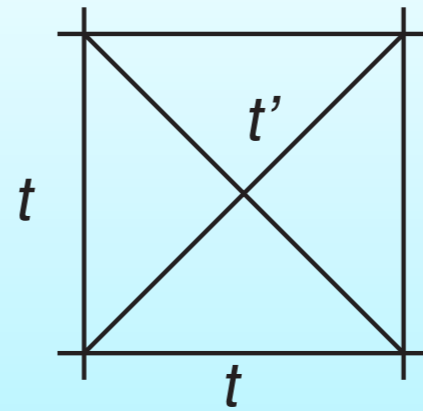
$$\tilde{c} \equiv \frac{1}{2\pi} \int_{\text{BZ}} \tilde{F}_{12}(k) d^2k$$

Also
 Intro

ge
 s,
 action

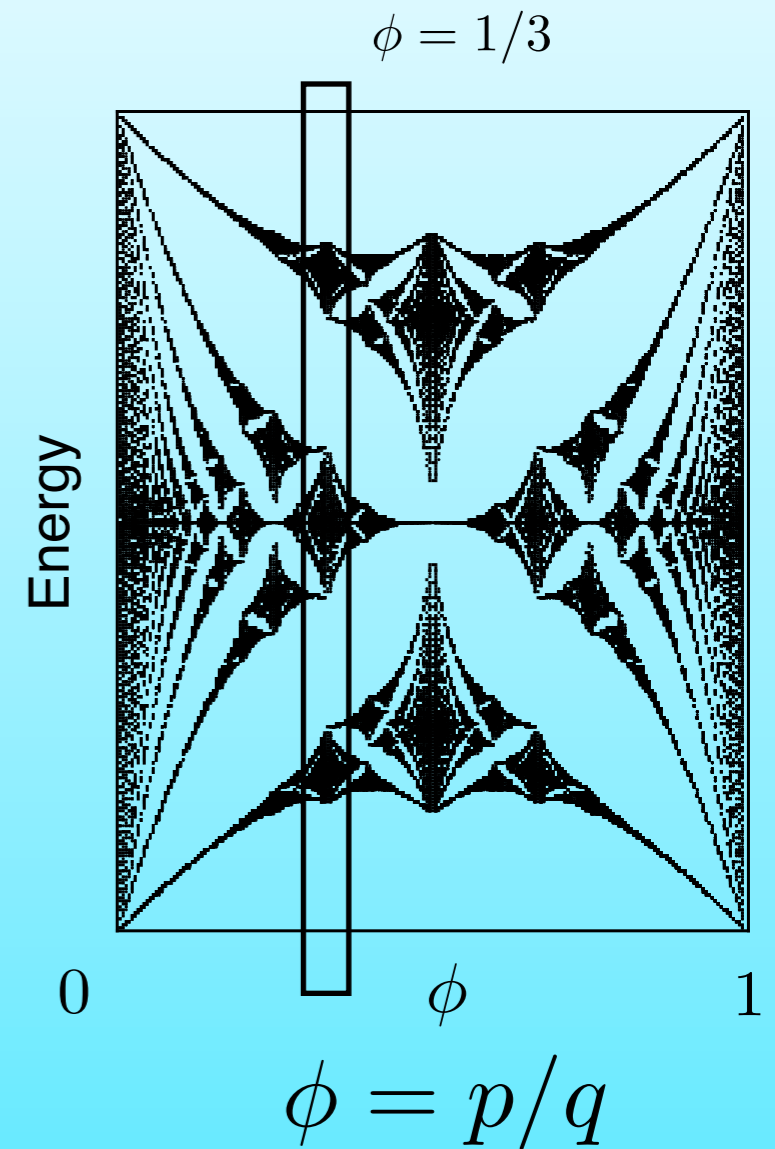
Ex.: 2D Bloch Electrons in a Magnetic Field

$\phi = 1/3$ second band
 $q = 3$



$$H(k) = \begin{pmatrix} -D_1 & -B_1 & 0 & \dots & -B_q^* e^{-iqk_x} \\ -B_1^* & -D_2 & -B_2 & & \\ 0 & -B_2^* & -D_3 & \ddots & \ddots \\ & \ddots & \ddots & \ddots & \\ -B_q e^{iqk_x} & 0 & & -B_{q-1}^* & -D_q \end{pmatrix}$$

$$H(k)|n(k)\rangle = E(k)|n(k)\rangle$$



$$D_j = t \cos(k_y + 2\pi\phi j)$$

$$B_j = t + 2t' \cos(k_y - 2\pi\phi(j + 1/2))$$

Admissibility and Critical Mesh Size

★ **Admissibility Condition:**

$$|\tilde{F}_{12}| < \pi$$

★ Need this for consistency

★ **Critical Mesh Size :**

$$N_B^C = \mathcal{O}(\tilde{c})$$

$$\tilde{c} = c \quad \text{if } N_B > N_B^C$$

★ To reproduce the one in the continuum

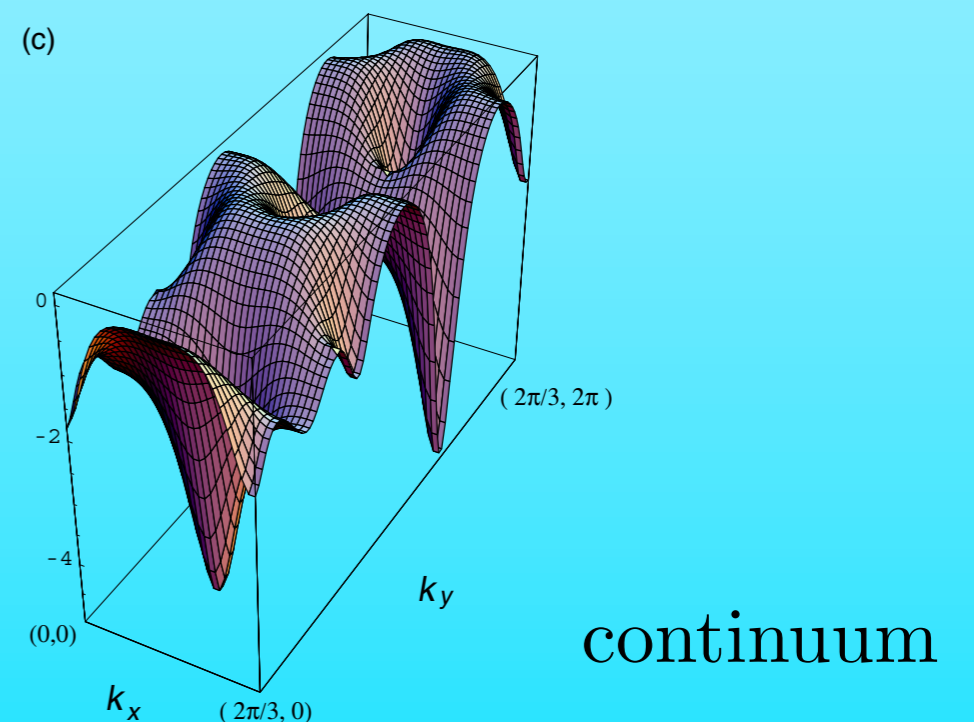
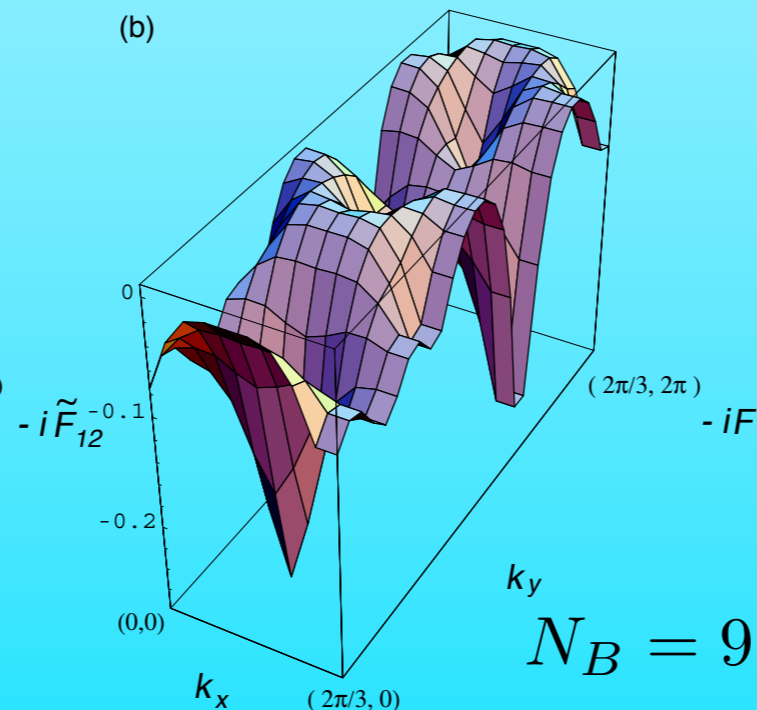
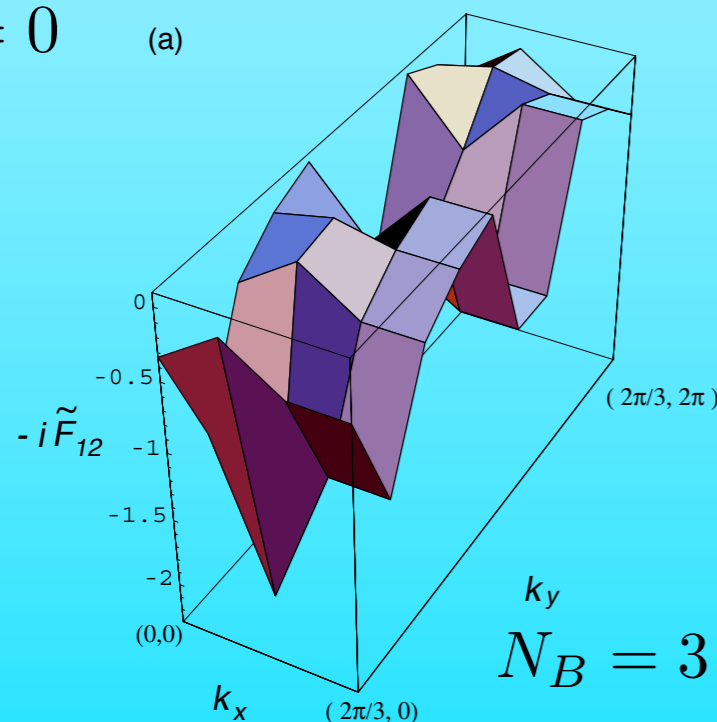
★ **Coarse discretization work quite well !!**

★ Advantage for Practical Numerical Calculation

$\tilde{c} = 2$ for both (a) and (b)

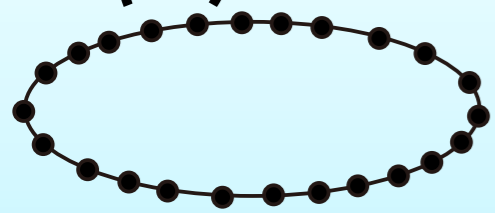
Lattice Field Strength \tilde{F}_{12} and Continuum Field Strength F_{12}

$t' = 0$



Numerical Evaluation of the Berry Phases (incl. non-Abelian)

(1) Discretize the periodic parameter space



$$x_0, x_1, \dots, x_N = x_0 \quad \theta_0 = 0, \theta_N = 2\pi$$
$$x_n = e^{i\theta_n} \quad \theta_{n+1} = \theta_n + \Delta\theta_n \quad \forall \Delta\theta_n \rightarrow 0$$

(2) Obtain eigen vectors

$$H(x_n)|\psi_n^i\rangle = E^i(x_n)|\psi_n^i\rangle$$

(3) Define Berry connection in a discretized form

$$A_n = \text{Im} \log \langle \psi_n | \psi_{n+1} \rangle$$

non-Abelian $A_n = \text{Im} \log \det D_n, \{D_n\}_{ij} = \langle \psi_n^i | \psi_{n+1}^j \rangle$

(4) Evaluate the Berry phase

$$\gamma = \sum_{n=0}^{N-1} A_n = \text{Im} \log \langle \psi_0 | \psi_1 \rangle \langle \psi_1 | \psi_2 \rangle \cdots (= \text{Im} \log \det D_1 D_2 \cdots D_n) \quad \text{non-Abelian}$$

Independent of the choice of the phase

$$|\psi_n\rangle \rightarrow |\psi_n\rangle' e^{i\Omega_n}$$

Gauge invariant

Luscher '82 (Lattice Gauge Theory)

after the discretization

King-Smith & Vanderbilt '93 (polarization in solids)

Convenient for Numerics

T. Fukui, H. Suzuki & YH '05 (Chern numbers)

Connection and Gauge Transformation

★ Berry's Connection $\Psi = (|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_M\rangle)$

$$\mathcal{A} = \Psi^\dagger d\Psi = \begin{pmatrix} \langle\psi_1| \\ \vdots \\ \langle\psi_M| \end{pmatrix} (|d\psi_1\rangle, \dots, |d\psi_M\rangle)$$

★ Gauge Transformation (Base Change)

$$\Psi' = \Psi\omega = (|\psi_1\rangle, |\psi_2\rangle, \dots, |\psi_M\rangle) \begin{pmatrix} \omega_{11} & \cdots & \omega_{1M} \\ \vdots & \ddots & \vdots \\ \omega_{M1} & \cdots & \omega_{MM} \end{pmatrix}$$

$$\Psi' = \Psi\omega$$

$$\mathcal{A}' = \Psi' d\Psi'$$

$$= \omega^{-1} \mathcal{A} \omega + \omega^{-1} d\omega$$

★ Field Strength $\mathcal{F} = d\mathcal{A} + \mathcal{A}\mathcal{A}$

$$\mathcal{F}' = \omega^{-1} \mathcal{F} \omega$$

$$\text{Tr } \mathcal{F} = \text{Tr } \mathcal{F}' = \text{Tr } d\mathcal{A}$$

Chern Numbers and Patch Work

★ Chern Numbers

$$C_S = \frac{1}{2\pi i} \int_S \text{Tr } \mathcal{F} = \frac{1}{2\pi i} \int_S \text{Tr } d\mathcal{A}$$

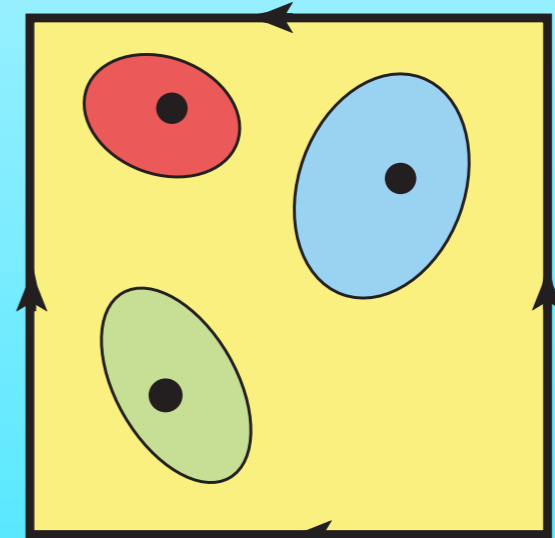
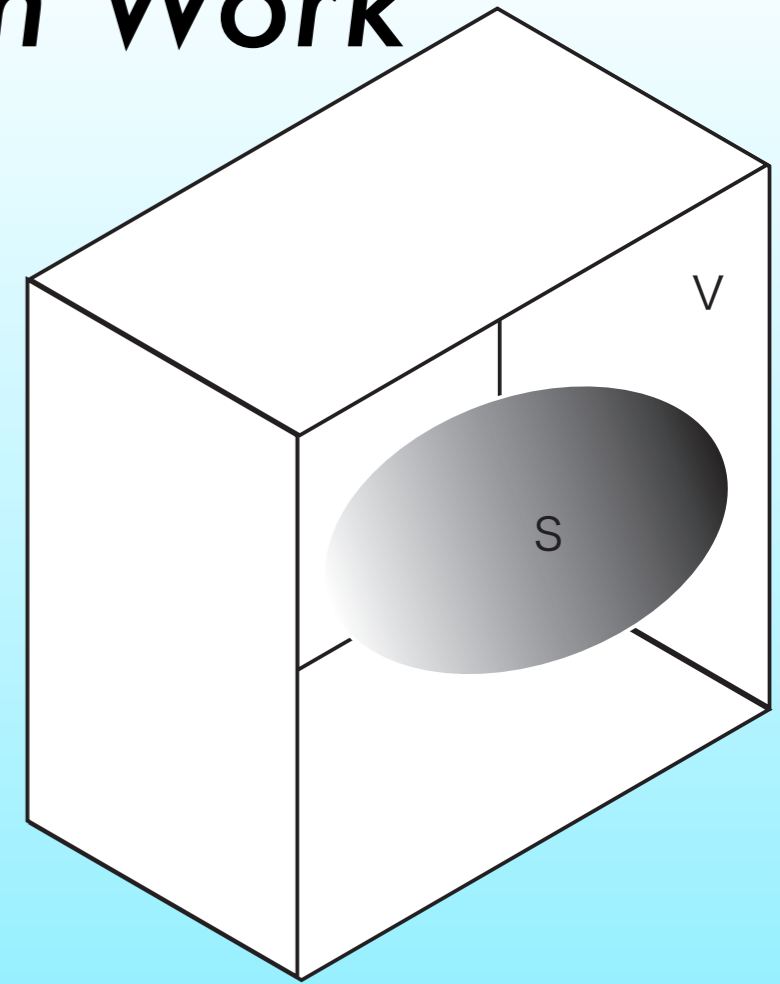
★ Patch Work on S

$$C_S = \frac{1}{2\pi i} \sum_R \int_{S_i} d\text{Tr } \mathcal{A}_R = \frac{1}{2\pi i} \sum_R \int_{\partial S_R} \text{Tr } \mathcal{A}_R$$

$$= \frac{1}{2\pi i} \sum_{R \geq 1} \int_{\partial S_R} \text{Tr } (\mathcal{A}_R - \mathcal{A}_0)$$

$$= \frac{1}{2\pi} \sum_{R \geq 1} \int_{\partial S_R} \text{Im Tr } \omega_{0R}^{-1} d\omega_{0R}$$

$$= \frac{1}{2\pi} \sum_{R \geq 1} \int_{\partial S_R} \text{Im Tr } d \log \omega_{0R}$$



$$\mathcal{A}(x) = \mathcal{A}_R(x), \quad x \in S_R, \quad S = \cup S_R, \quad R = 0, 1, 2, \dots$$

$$\Psi_R = \Psi_0 \omega_{0R}$$

$$\mathcal{A}_R = \omega_{0R}^{-1} \mathcal{A}_0 \omega_{0R} + \omega_{0R}^{-1} d\omega_{0R}$$

Non Abelian Chern Number on Lattice

★ *The Lattice Formulation is also applicable!*

$$U_\mu(k_\ell) \equiv \langle n(k_\ell) | n(k_\ell + \hat{\mu}) \rangle / \mathcal{N}_\mu(k_\ell)$$

$$U_\mu(k_\ell) : \quad \mathcal{N}_\mu(k_\ell) = |\langle n(k_\ell) | n(k_\ell + \hat{\mu}) \rangle|$$



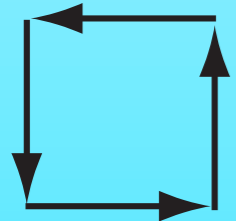
$$U_\mu(k_\ell) = \det \psi^\dagger(k_\ell) \psi(k_\ell + \hat{\mu}) / \mathcal{N}_\mu(k_\ell)$$

$$\mathcal{N}_\mu(k_\ell) = |\det \psi^\dagger(k_\ell) \psi(k_\ell + \hat{\mu})|$$

$$\tilde{F}_{12}(k_\ell)$$

$$\psi = (|n_1\rangle, \dots, |n_M\rangle)$$

$$H|n_j\rangle = E_j(k)|n_j\rangle$$



: The same as the Abelian case

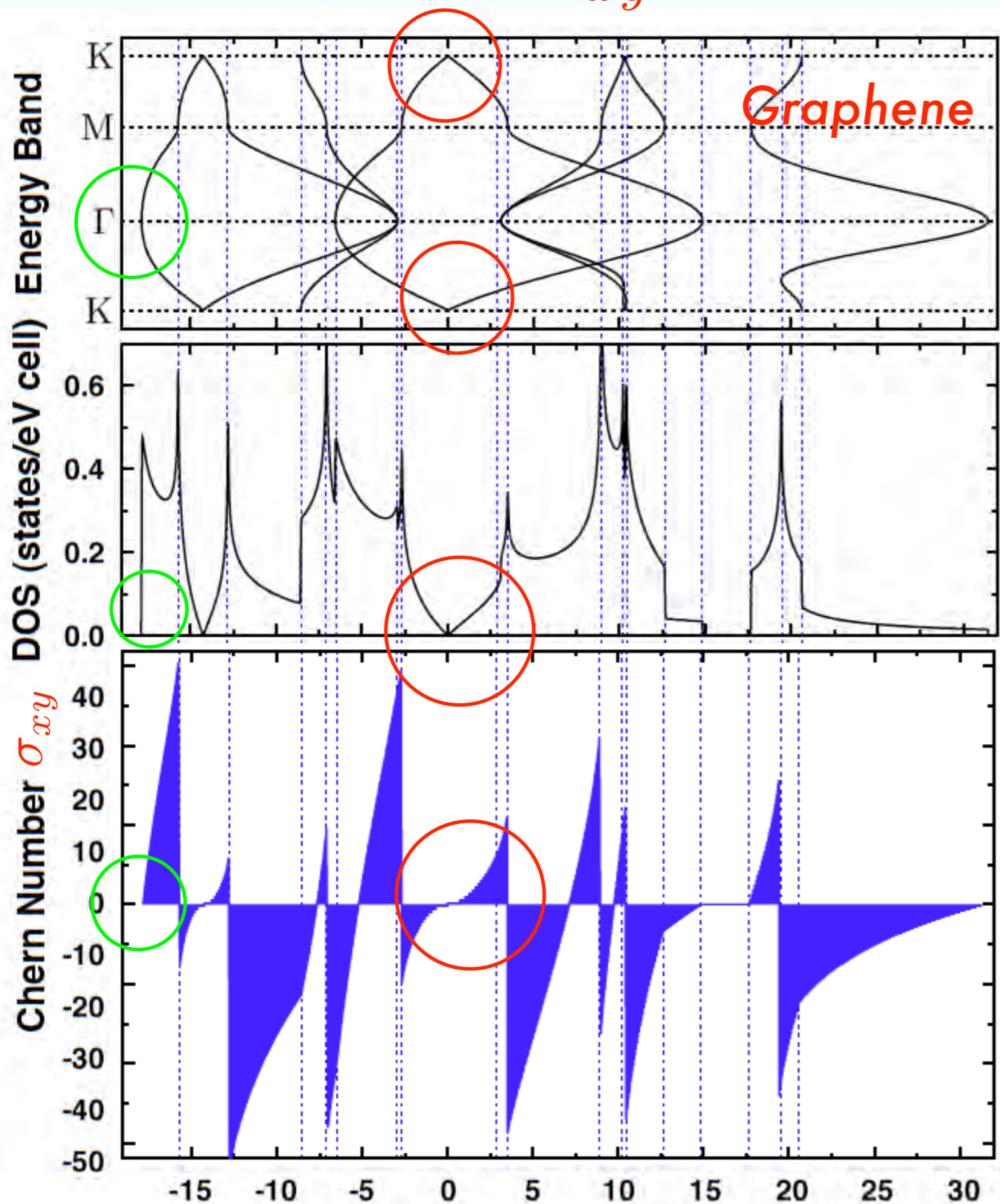
$$\psi^\dagger \psi = \mathbf{I}_M$$

$$\tilde{c} = \frac{1}{2\pi i} \sum_\ell \tilde{F}_{12}(k_\ell) \xrightarrow{N_B \rightarrow \infty} c = \frac{1}{2\pi i} \int \text{Tr} dA$$

$$A = \psi^\dagger d\psi$$

Chern numbers (σ_{xy}) based on Realistic Band Calc.

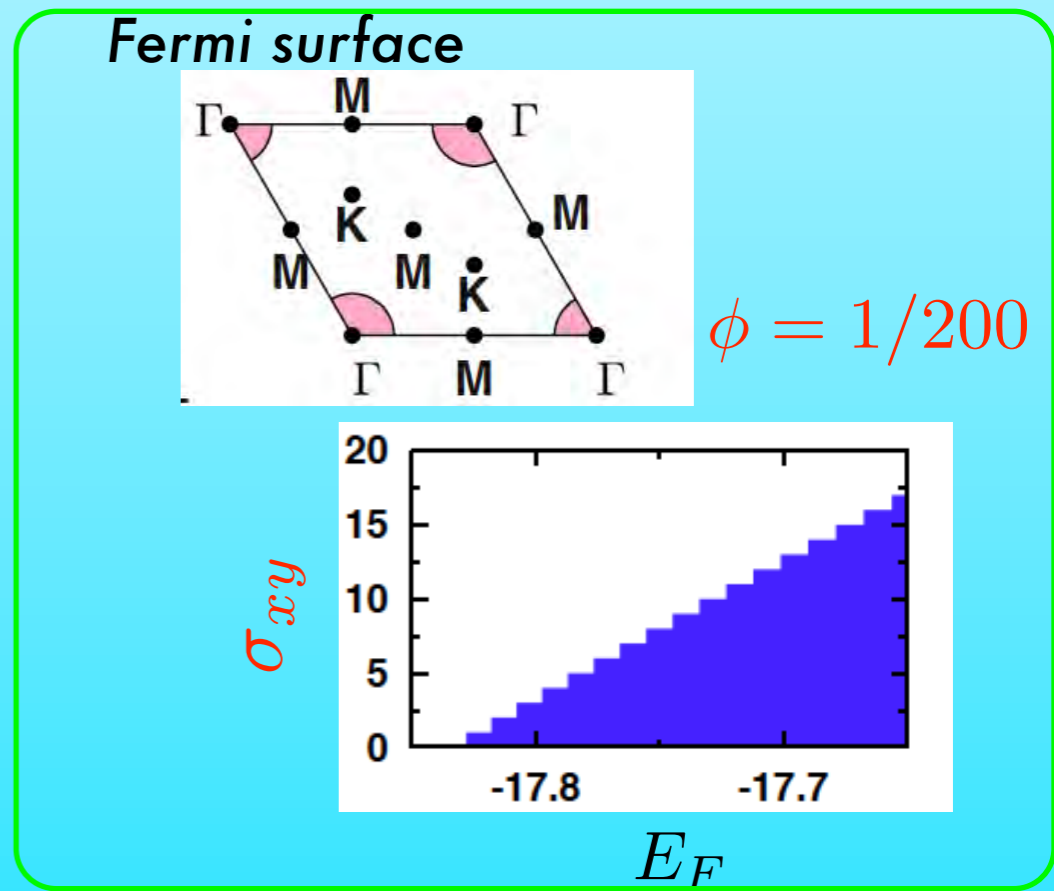
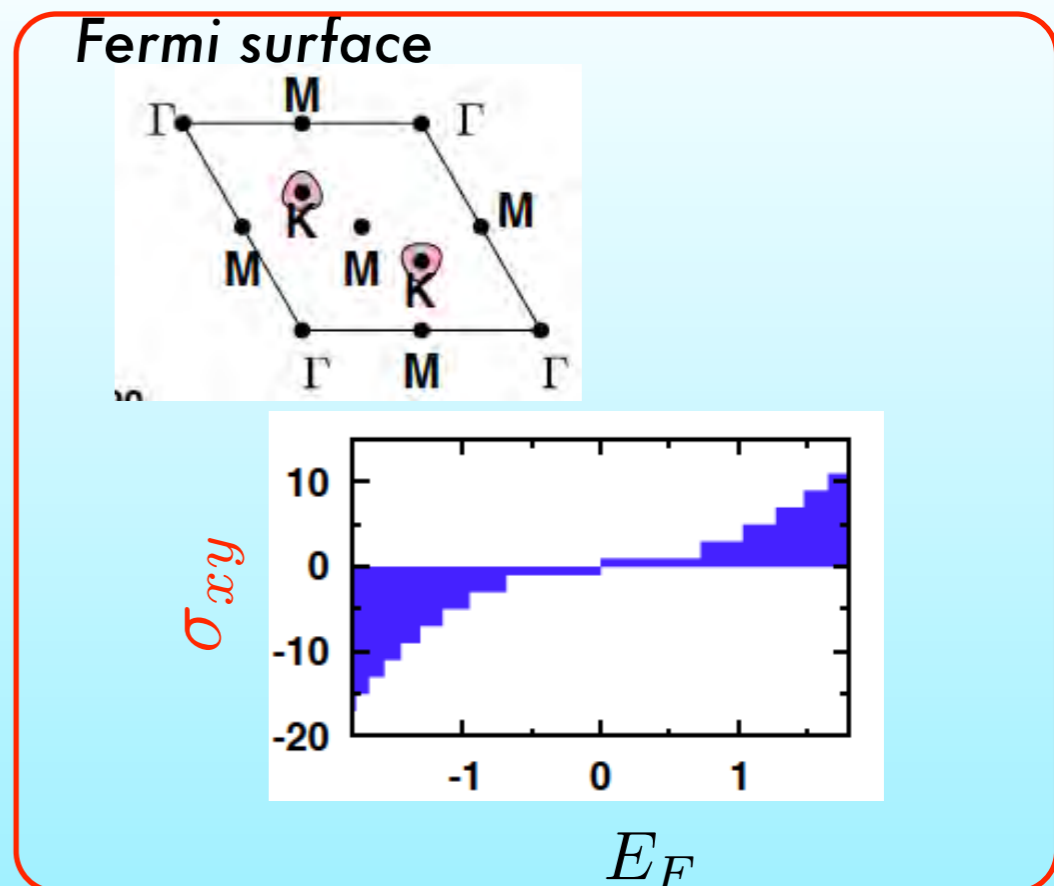
Berry phases,...



quantized everywhere

Energy (eV)

M.Arai and Y.Hatsugai, Phys.Rev. B79, 075429 (2009)



END