

TKNN formula for general Hamiltonian in odd dimensions

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arXiv:1903.11852

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1. Introduction

Topological insulator is interesting
(particularly to lattice theorists)

➤ **Interesting physics from non-trivial topology**

Bulk: insulator

Topology guarantees edge modes

Surface: metal

(Bulk-Edge correspondence)

➤ **Close relationship to domain-wall fermion**

New knowledge of topological matter

➔ new hints to lattice fermions by Domain-wall fermion

example: Gapped symmetric phase by 4-fermi interaction

➔ Chiral gauge theory on the lattice

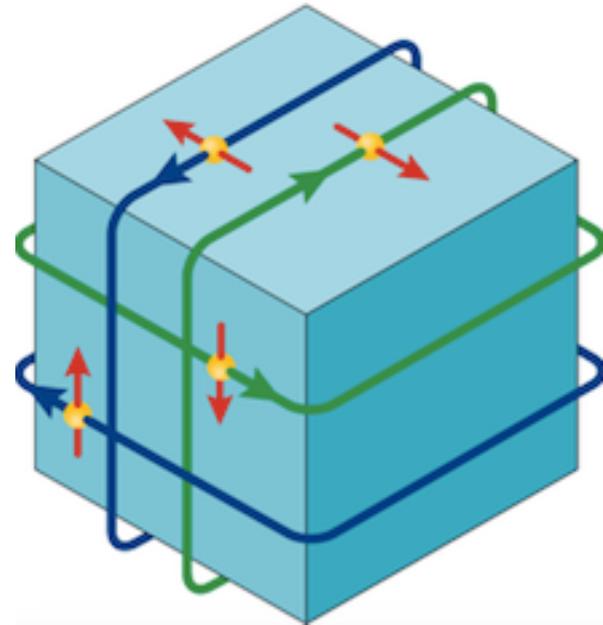


Figure from Tokura et al.
Nature Reviews Physics vol 1, 126 (2019)

Characterization of topological insulator

Microscopic approach

TKNN formula

Thouless, Kohmoto, . Nightingale, . den Nijs

Study the wavefunction of free fermion

Applied to various different free systems
(higher dim, higher symmetry)

Looks rather technical (at least to me)

Applicable only to free fermion systems

Field theory approach

Callan-Harvey

K. Ishikawa 1984, H. So 1985, Golterman, Jansen, Kaplan 1993

Study the effective action with gauge field

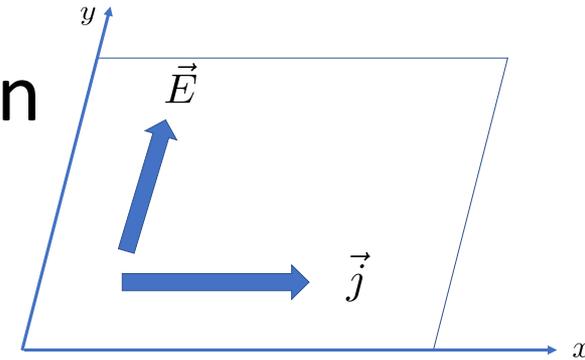
Conceptually simple :
bulk-edge correspondence = anomaly cancellation

Applicable also to interacting fermion systems

TKNN formula Thouless, Kohmoto, . Nightingale, . den Nijs

2+1 dim system with Parity Violation

Hall current perpendicular to Electric field



$$\langle j_x \rangle_E = \sigma_{xy} E_y$$



- 1) Kubo formula from perturbation theory
- 2) Formulae in quantum mechanics

$$\sigma_{xy} = \frac{e^2}{2\pi} \int \frac{d^2 \vec{p}}{2\pi} \sum_a \epsilon^{ij} \frac{\partial}{\partial p^i} \mathcal{A}_j^{(a)}(\vec{p})$$

Chern number

$|a, \vec{p}\rangle$, a : label for band,
 \vec{p} : momentum

$$\mathcal{A}_i^{(a)}(\vec{p}) \equiv -i \langle a, \vec{p} | \frac{\partial}{\partial p^i} | a, \vec{p} \rangle$$

Berry connection

Field Theory approach

Integrating out massive fermions in 3-dimensions

$$S_{\text{eff}}(A) = ic_{cs} S_{cs}(A) + \dots \qquad S_{\text{eff}}(A) \equiv \ln \left[\int D\psi D\psi^\dagger e^{-\int \psi^\dagger (iD_0 - H(A)) \psi} \right]$$



Chern-Simons action

$$S_{\text{eff}}(A) = ic_{cs} \int d^3x \epsilon^{\mu\nu\lambda} A_\mu \partial_\nu A_\lambda$$

Hall conductivity is given by the Chern-Simons coupling c_{cs}

$$\langle j_i \rangle = \frac{\delta}{i\delta A_i} S_{\text{eff}}(A) = 2c_{cs} \epsilon^{i\nu\lambda} \partial_\nu A_\lambda = 2c_{cs} \epsilon^{ij} E_j$$

For simple or special cases,

1) explicit 1-loop calculation, 2) Ward-Takahashi identity $\partial_\mu S_F^{-1}(p) = -i\Gamma_\mu(k, p) |_{k=0}$

“Winding number” expression of Chern-Simons coupling

$$c_{cs} = -\frac{\epsilon^{\alpha_0\beta_1\alpha_1}}{2 \cdot 3!} \int \frac{d^3 p}{(2\pi)^3} \text{Tr} [S(p) \partial_{\alpha_0} S^{-1}(p) S(p) \partial_{\beta_1} S^{-1}(p) S(p) \partial_{\alpha_1} S^{-1}(p)]$$

K. Ishikawa 1984, H. So 1985, Golterman, Jansen, Kaplan 1993

Topological invariant of a map $(p^0, \vec{p}) \in R \times T^2 \rightarrow S_F(p)$

Question

Two topological characterizations are identical?

In some specific cases, yes.

How generally identical and why ?

We prove the equivalence for general Hamiltonians bilinear in fermion in $D=2+1$ and $D=4+1$ dimensions.

Outline

- ✓ □ 1. Introduction
- 2. Equivalence for general Hamiltonian
 - 1. The Setup and outline of the proof
 - 2. Fermion-loop expression \rightarrow Winding number expression
 - 3. Winding number expression \rightarrow TKNN formula
- 3. Summary

2. Equivalence for general Hamiltonian

Fukaya, T.O., Yamaguchi, Xi
arXiv:1903.11852

2-1. The Setup

Gapped fermion system in $D=2n+1$ dimensions.

Fermions on $2n$ dim lattice with continuous time in Euclidean space

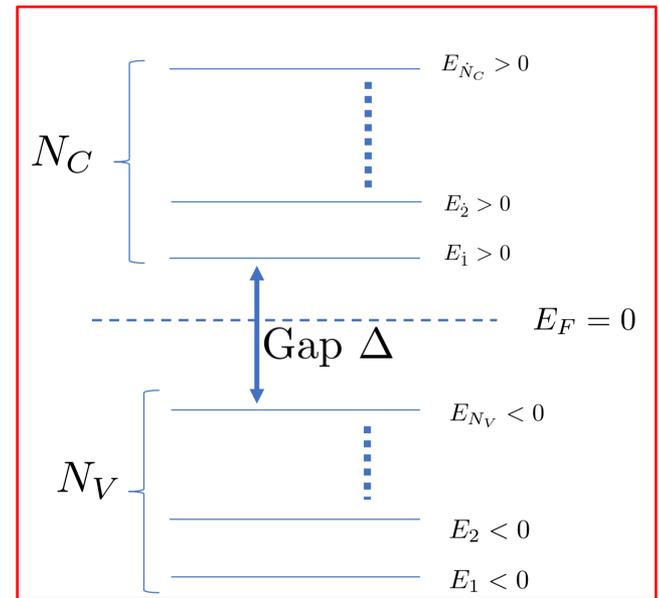
$$S_E = \int dt \sum_{\vec{r}} \psi^\dagger(t, \vec{r}) \left[\frac{\partial}{\partial t} + iA_0 + H(\vec{A}) \right] \psi(t, \vec{r})$$

$H(\vec{A}) \Big|_{\vec{A}=0}$: translational inv. \rightarrow band structure

ψ, ψ^\dagger can have many internal DOF
 \rightarrow Many bands

No particular structure is assumed
 such as relativistic fermion, or Wilson fermion,

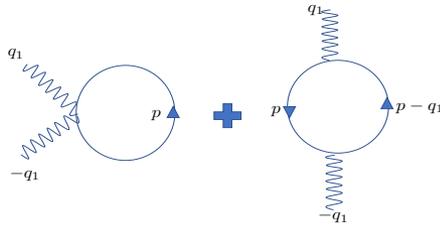
Energy eigenstates for fixed \vec{p}



N_V Valence bands
 N_C Conduction bands
 Δ : Gap

Outline of the proof

fermion loop expression of c_{CS}



Generalized Ward-Takahashi identities

winding number expression of c_{CS}

$$c_{CS} = \frac{(-i)^2 \epsilon_{\alpha_0 \beta_1 \alpha_1}}{2!3!} \int \frac{dp_0}{2\pi} \int_{\text{BZ}} \frac{d^2 p}{(2\pi)^2} \\ \times \text{Tr} \left[S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_0}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_1}} \right]$$

Energy eigenstate expression & p_0 integration

TKNN formula

$$c_{CS} \propto \sum_a \int \frac{d^2 \vec{p}}{2\pi} \epsilon^{ij} \partial_i \mathcal{A}_j^{(a)}$$

2-2. Fermion-loop expression \rightarrow Winding number expression

$$S_{\text{eff}}(A) = \cdots + i c_{CS} S_{CS}(A) + \cdots$$

$$S_{CS}(A) = \int d^{2n+1}x \epsilon_{\alpha_0 \beta_1 \alpha_1 \cdots \beta_n \alpha_n} A_{\alpha_0} \partial_{\beta_1} A_{\alpha_1} \cdots \partial_{\beta_n} A_{\alpha_n}$$

c_{CS} can be obtained by differentiating the effective action as

$$c_{CS} = \frac{(-i)^{n+1} \epsilon_{\alpha_0 \beta_1 \alpha_1 \cdots \beta_n \alpha_n}}{(n+1)!(2n+1)!} \left(\frac{\partial}{\partial q_1} \right)_{\beta_1} \cdots \left(\frac{\partial}{\partial q_n} \right)_{\beta_n} \\ \times \prod_{i=1}^n \int d^{2n+1}x_i e^{iq_i x_i} \frac{\delta^{n+1} S_{\text{eff}}(A)}{\delta A_{\alpha_0}(x_0) \delta A_{\alpha_1}(x_1) \cdots \delta A_{\alpha_n}(x_n)} \Big|_{A=0, q_i=0}$$

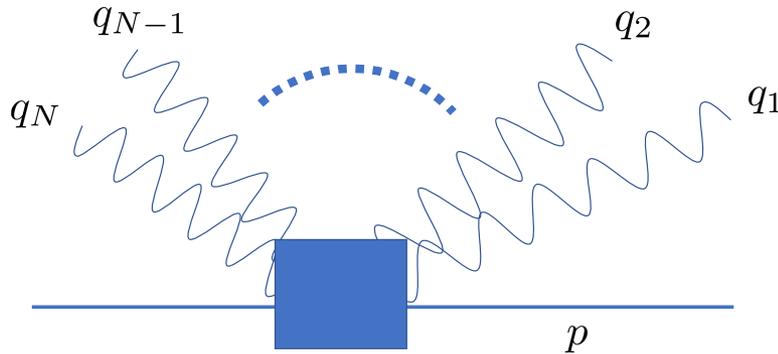


Fermion 1-loop diagram with $n+1$ external photons

For general Hamiltonian,

Feynman rule can have fermion-fermion-multiphoton vertices

$$\Gamma^{(n)}[q_N, \alpha_N; \cdots; q_1, \alpha_1; p]$$



➔ 1-loop n-point function from several diagrams in general.

D=2+1 case

$$c_{cs} = -\frac{(-i)^2 \epsilon_{\alpha_0 \beta_1 \alpha_1}}{2!3!} \int \frac{d^3 p}{(2\pi)^3} \left(\frac{\partial}{\partial q_1} \right)_{\beta_1} \left\{ \text{Tr} \left[S_F(p) \Gamma^{(2)}[-q_1, \alpha_0; q_1, \alpha_1; p] \right] + \text{Tr} \left[S_F(p - q_1) \Gamma^{(1)}[-q_1, \alpha_0; p] S_F(p) \Gamma^{(1)}[q_1, \alpha_1; p - q_1] \right] \right\} \Big|_{q_1=0}$$

↕

$$X \equiv \epsilon^{\alpha_0 \beta_1 \alpha_1} \left(\frac{\partial}{\partial q_1} \right)_{\beta_1} \left[\text{Diagram 1} + \text{Diagram 2} \right]$$

The diagram illustrates the Feynman diagrams corresponding to the terms in the trace. The first diagram shows a fermion loop with momentum p and two external wavy lines with momenta q_1 and $-q_1$ and indices α_1 and α_0 . The second diagram shows a fermion loop with momentum p and two external wavy lines with momenta q_1 and $-q_1$ and indices α_1 and α_0 , but the wavy lines are attached to the loop at different vertices.

Naively, simplest Ward-Takahashi identity reduce the fermion loop expression into winding number expression

$$\partial_\mu S_F^{-1}(p) = -i\Gamma_\mu(k, p) |_{k=0}$$

K. Ishikawa 1984, H. So 1985, Golterman, Jansen, Kaplan 1993

However, two new contributions in general case

1. Multi-photon vertex contribution \rightarrow non-zero
2. Momentum derivative of the vertex function \rightarrow non-zero

corrections to the winding number expression!

New Ward-Takahashi identity

$$\left. \frac{\partial^2 \Gamma^{(1)}[k, \mu; p]}{\partial k_\nu \partial p_\lambda} \right|_{k=0} = \left. \frac{\partial \Gamma^{(2)}[k, \mu; 0, \lambda; p]}{\partial k_\nu} \right|_{k=0} = \left. \frac{\partial \Gamma^{(2)}[0, \lambda; l, \mu; p]}{\partial l_\nu} \right|_{l=0}$$

1st derivative of the two-photon vertex with respect to momentum is related to 2nd derivative of the single photon vertex.



Correction terms to 1-loop expression is shown to be total derivatives and vanish.

Using these Ward-Takahashi identities, one can rewrite the integrand X as

$$X = \epsilon^{\alpha_0 \beta_1 \alpha_1} \frac{\partial}{\partial p_{\alpha_0}} \text{Tr} \left(2S_F(p) \frac{\partial \Gamma^{(1)}[q_1, \alpha_1; p]}{\partial q_{\beta_1}} \right) \Big|_{q=0} + \epsilon^{\alpha_0 \beta_1 \alpha_1} \left(S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_0}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_1}} \right)$$

Therefore, additional contributions add up to a total derivative.

Thus, for general Hamiltonian, we obtain

$$c_{\text{CS}} = \frac{(-i)^2 \epsilon_{\alpha_0 \beta_1 \alpha_1}}{2!3!} \int \frac{dp_0}{2\pi} \int_{\text{BZ}} \frac{d^2 p}{(2\pi)^2} \times \text{Tr} \left[S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_0}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_1}} \right]$$

D=4+1 case

Chern-Simons coupling is obtained from 3-point 1-loop diagrams.
A lot of extra terms appear.

However, one can derive new 3rd order WT-identity from formal expansion of the action in terms of covariant derivatives as

$$\left. \frac{\partial^2 \Gamma^{(3)}[q, \mu; r, \nu; s, \lambda; p]}{\partial q_\alpha \partial r_\beta} \right|_{q,r,s=0} = \left. \frac{\partial^3 \Gamma^{(2)}[q, \mu; r, \nu; p]}{\partial q_\alpha \partial r_\beta \partial p_\lambda} \right|_{q,r=0}$$

$$c_{cs} = -\frac{(-i)^3 \cdot 2}{3!5!} \int \frac{d^5 p}{(2\pi)^5} \epsilon_{\alpha_0 \beta_1 \alpha_1 \beta_2 \alpha_2} \\ \times \text{Tr} \left[S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_0}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_1}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\beta_2}} S_F(p) \frac{\partial S_F^{-1}(p)}{\partial p_{\alpha_2}} \right]$$

2-3 Winding number \rightarrow TKNN formula

This part was essentially already given by

Qi, Hughes, Zhang, Phys. Rev. B 78, 195424, 2008

Idea : Evaluate the winding number expression as follows

1. Rewrite the fermion propagator using eigenstates

$$S(p) = \sum_{\alpha} |\alpha, \vec{p}\rangle \frac{1}{ip^0 + E_{\alpha}(\vec{p})} \langle \alpha, \vec{p}|$$

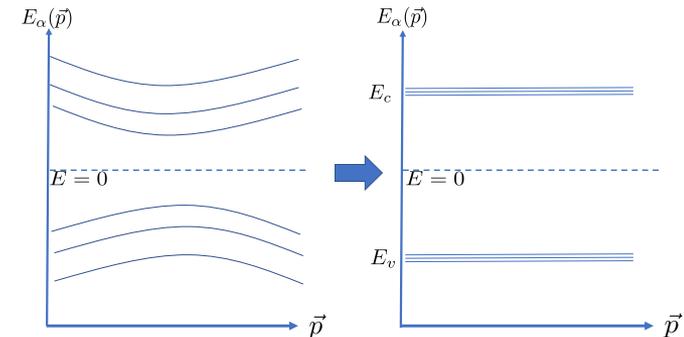
2. Continuously deform only the eigenvalues to degenerate flat band

$$E_{\alpha}(\vec{p}) (< 0) \longrightarrow E_v = \text{constant}$$

$$E_{\alpha}(\vec{p}) (> 0) \longrightarrow E_c = \text{constant}$$

$|a\rangle$ ($a = 1, \dots, N_v$) : valence bands

$|\dot{a}\rangle$ ($\dot{a} = 1, \dots, N_c$) : conduction bands



3. Carry out momentum integral over p^0

Step 1

Inserting complete set of energies eigenstates, one obtains

$$c_{cs} = \frac{n!(-i)^{n+2}}{(n+1)!(2n)!} \int \frac{d^{2n}p}{(2\pi)^{2n}} J$$

$$J = \sum_{\alpha_1, \dots, \alpha_{2n}} \epsilon^{i_1 i_2 \dots i_{2n}} \int \frac{dp^0}{2\pi} \frac{\langle \alpha_1 | \partial_{i_1} H | \alpha_2 \rangle \langle \alpha_2 | \partial_{i_2} H | \alpha_3 \rangle \dots \langle \alpha_{2n} | \partial_{i_{2n}} H | \alpha_1 \rangle}{(ip^0 + E_{\alpha_1})^2 (ip^0 + E_{\alpha_2}) \dots (ip^0 + E_{\alpha_{2n}})}$$

Useful formulae

$$\langle a(\vec{p}) | \partial_\mu H(\vec{p}) | b(\vec{p}) \rangle = 0, \quad \langle \dot{a}(\vec{p}) | \partial_\mu H(\vec{p}) | \dot{b}(\vec{p}) \rangle = 0,$$

$$\langle a(\vec{p}) | \partial_\mu H(\vec{p}) | \dot{b}(\vec{p}) \rangle = (E_c - E_v) \langle a | \partial_\mu \dot{b} \rangle,$$

$$\langle \dot{a}(\vec{p}) | \partial_\mu H(\vec{p}) | b(\vec{p}) \rangle = -(E_c - E_v) \langle \dot{a} | \partial_\mu b \rangle,$$

$$(a, b = 1, \dots, N_v, \quad \dot{a}, \dot{b} = 1, \dots, N_c).$$

shows that inserted states should be valence and conduction band appearing alternately.

Step 3

p^0 integration can be easily carried out by Cauchy integral

$$J = \sum_{a_1, \dots, a_n=1}^{N_v} \sum_{\dot{a}_1, \dots, \dot{a}_n=1}^{N_c} \epsilon^{i_1 j_1 \dots i_n j_n} (-1)^{n+1} \frac{(2n)!}{(n!)^2} \\ \times \langle a_1 | \partial_{i_1} \dot{a}_1 \rangle \langle \dot{a}_1 | \partial_{j_1} a_2 \rangle \times \dots \times \langle a_n | \partial_{i_n} \dot{a}_n \rangle \langle \dot{a}_n | \partial_{j_n} a_1 \rangle.$$

Berry connection

Define the Berry connection as

$$\mathcal{A}^{ab} \equiv \mathcal{A}_\mu^{ab} dp^\mu = -i \langle a | \partial_\mu b \rangle dp^\mu = -i \langle a | db \rangle$$



$$\mathcal{F}^{ab} \equiv (d\mathcal{A} + i\mathcal{A}\mathcal{A})^{ab}$$

$$= -\langle da | db \rangle + i \sum_{c=1}^{N_v} (-i) \langle a | dc \rangle (-i) \langle c | db \rangle$$

Inserting complete set

$$\mathbf{1} = \sum_{c=1}^{N_v} |c\rangle \langle c| + \sum_{\dot{c}=1}^{N_c} |\dot{c}\rangle \langle \dot{c}|$$



$$\mathcal{F}^{ab} = i \sum_{\dot{c}=1}^{N_c} \langle a | d\dot{c} \rangle \langle \dot{c} | db \rangle$$

This product gives Berry curvature!

Using $\mathcal{F}^{ab} = i \sum_{\dot{c}=1}^{N_c} \langle a|d\dot{c}\rangle \langle \dot{c}|db\rangle$, one can rewrite the integrand J using only the product of Berry curvature

Inserting this expression into c_{cs} using J, and using the definition of the Berry curvature one obtains

$$c_{cs} \equiv \frac{k}{(n+1)!(2\pi)^n} = \frac{(-1)^n}{(n+1)!(2\pi)^n} \int_{BZ} \text{ch}_n(\mathcal{A}),$$

$$\text{ch}_n(\mathcal{A}) = \frac{1}{n!} \frac{1}{(2\pi)^n} \text{tr}(\mathcal{F}^n)$$

This result shows that

Chern-Simons level in field theory approach
and

Chern number in microscopic approach (TKNN)
are identical for general Hamiltonian bilinear in
fermion for $D=2+1, 4+1$ dimensions.

5. Summary

- We have shown microscopic approach (TKNN) and field theory approach give identical topological number for general Hamiltonian bilinear in fermion.
- A series of Ward-Takahashi identities are crucial to show the equivalence.
- No other details beyond gauge symmetry (such as existence of relativistic field theory at low energy) is needed.

- In 4+1 dimensions, there are two independent Chern numbers. However, only a particular Chern number appeared.
- This means that topological classification in microscopic approach may be finer, or those detailed structure may not be robust.
- It would be interesting to see similar equivalence holds or not for other cases such as systems with higher symmetry or systems with interacting fermions.

Backup Slides

Formal expansions of propagator and vertices

Using the coefficients M ,

$$S_F^{-1}(p) = \sum_{n=0}^{\infty} M_{\mu_1 \dots \mu_n} \prod_{i=1}^n (ip_{\mu_i})$$

$$\Gamma^{(1)}[k, \mu; p] = -i \sum_{n=1}^{\infty} \sum_{a=1}^n M_{\mu_1 \dots \mu_{a-1} \mu \mu_{a+1} \dots \mu_n} \prod_{i=1}^{a-1} (i(p+k)_{\mu_i}) \prod_{i=a+1}^n (ip_{\mu_i})$$

$$\begin{aligned} \Gamma^{(2)}[k, \mu; l, \nu; p] &= -i^2 \sum_{n=1}^{\infty} \sum_{\substack{a,b=1 \\ a < b}}^n M_{\mu_1 \dots \mu_{a-1} \mu \mu_{a+1} \dots \mu_{b-1} \nu \mu_{b+1} \dots \mu_n} \prod_{i=1}^{a-1} (i(p+k+l)_{\mu_i}) \prod_{i=a+1}^{b-1} (i(p+l)_{\mu_i}) \prod_{i=b+1}^n (ip_{\mu_i}) \\ &- i^2 \sum_{n=1}^{\infty} \sum_{\substack{a,b=1 \\ a < b}}^n M_{\mu_1 \dots \mu_{a-1} \nu \mu_{a+1} \dots \mu_{b-1} \mu \mu_{b+1} \dots \mu_n} \prod_{i=1}^{a-1} (i(p+k+l)_{\mu_i}) \prod_{i=a+1}^{b-1} (i(p+k)_{\mu_i}) \prod_{i=b+1}^n (ip_{\mu_i}) \end{aligned}$$

New Ward-Takahashi identities

Gauge invariant lattice action can be formally expanded by infinite series of covariant derivatives.

Example:
$$\psi^\dagger(t, \vec{x}) e^{i \int_{\vec{x}}^{\vec{x} + a\vec{\mu}} d\vec{r}' \cdot \vec{A}(\vec{r}')} \psi(t, \vec{x} + a\vec{\mu}) = \psi^\dagger(t, \vec{x}) \sum_{n=0}^{\infty} \frac{a^n}{n!} (D_{\vec{\mu}}^n \psi)(t, \vec{x})$$

Therefore, formally action can be expressed as

$$S = \int dt \sum_{\vec{x}} \sum_{n=0}^{\infty} \psi^\dagger(t, \vec{x}) M_{\mu_1 \dots \mu_n} (D_{\mu_1} \dots D_{\mu_n} \psi)(t, \vec{x})$$

Same coefficient M appear in propagator and vertices

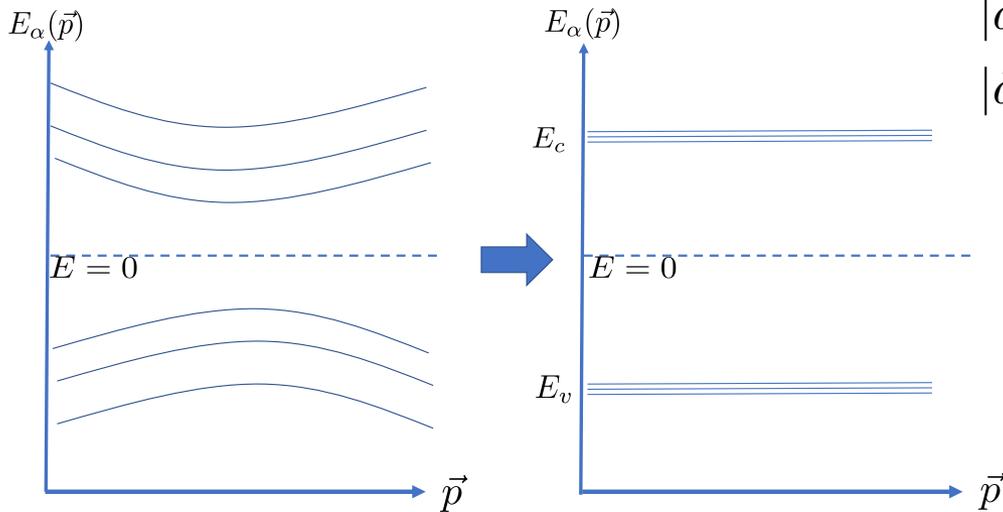
Step 2

Continuously deform Hamiltonian by changing only the eigenvalues keeping the gap to degenerate flat band.

$$H(\vec{p}) \equiv \sum_{a=1}^{N_v} E_a(\vec{p}) |a(\vec{p})\rangle \langle a(\vec{p})| + \sum_{\dot{b}=1}^{N_c} E_{\dot{b}}(\vec{p}) |\dot{b}(\vec{p})\rangle \langle \dot{b}(\vec{p})|$$



$$H_{\text{new}}(\vec{p}) = E_v \sum_{a=1}^{N_v} |a(\vec{p})\rangle \langle a(\vec{p})| + E_c \sum_{\dot{b}=1}^{N_c} |\dot{b}(\vec{p})\rangle \langle \dot{b}(\vec{p})|$$



$|a\rangle$ ($a = 1, \dots, N_v$) : valence bands

$|\dot{a}\rangle$ ($\dot{a} = 1, \dots, N_c$) : conduction bands