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Topological Properties of Non-Periodic Kronig-Penney Model

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Outline

- 1. Introduction***
- 2. Review of Topology in Condensed Matter Physics***
- 3. Main part : My Research Topic***



1. Introduction

1.1. Self Introduction

1.2. Why I came here?

1.3. My previous study (Not research)

1.3.1. Topological Insulator

1.3.2. Bose-Hubbard Model

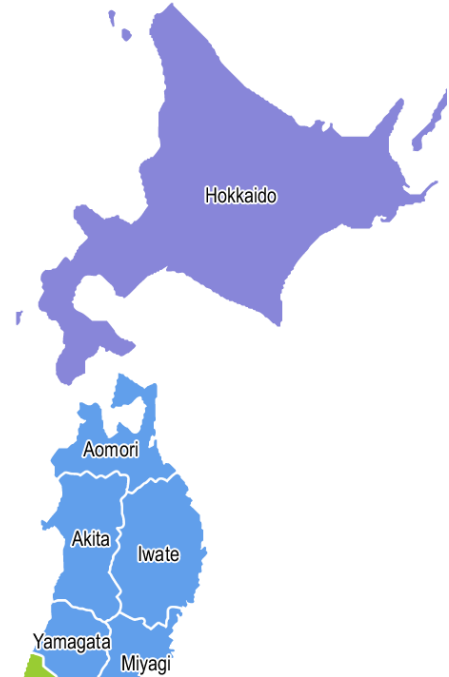
1.3.4. Kosterlitz-Thouless transition

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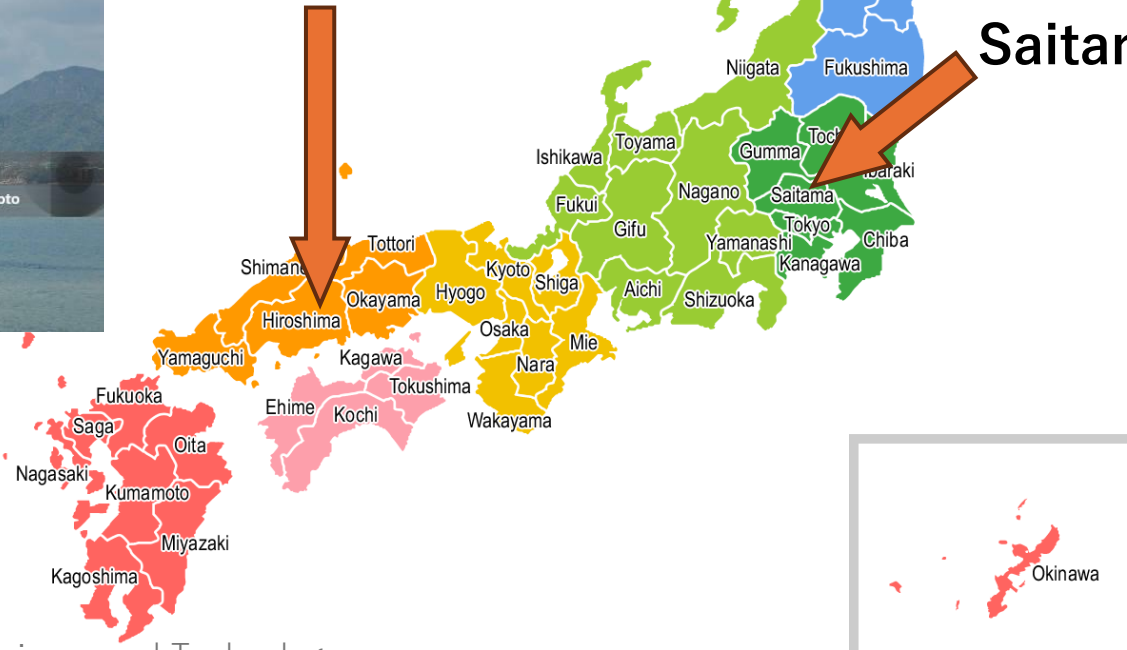


Hiroshima:



Hiroshima

Saitama



Saitama:



Self Introduction

- ✓ Research Unit in Hiroshima University → **Condensed matter Theory Group**
- ✓ Our Unit member are especially interested in **Topological Phenomena**

PI (supervisor): Prof. Yasuhiro Tada

- Superconductivity
- Quantum criticality
- Dirac electrons
- Heavy fermions
- Topological systems
- Quantum magnets
- Spin liquids

M2, 1 person: Quantum Spin liquids

M1, 1 person: Fractional quantum Hall effect

B4, 4 people: Undecided

※

M2 = 2nd year master student

M1 = 1st year master student

B4 = 4th year bachelor student

In Japan Graduate school

= two years mater degrees + three years Ph.D. degrees



Why I came here?

Last year, I took a lecture titled

An Introduction to Ultracold Atom Physics for Condensed Matter Physics and Quantum Computation

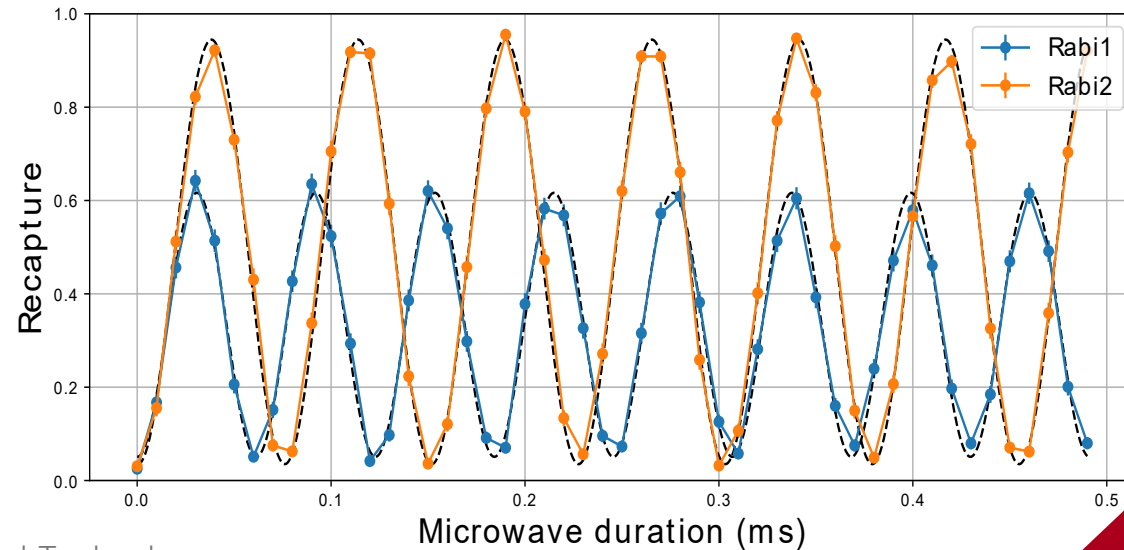
by Prof. Tomita (Institute for Molecular Science Ohmori group)

→ I started to have interested in Ultracold Atom Physics

+

I knew the OIST Research Internship program and found the QSU group

I also, I went to Institute for Molecular Science Ohmori group for three days and did a easy experiment (observation of Rabi oscillation) based on Prof. Tomita's instruction.





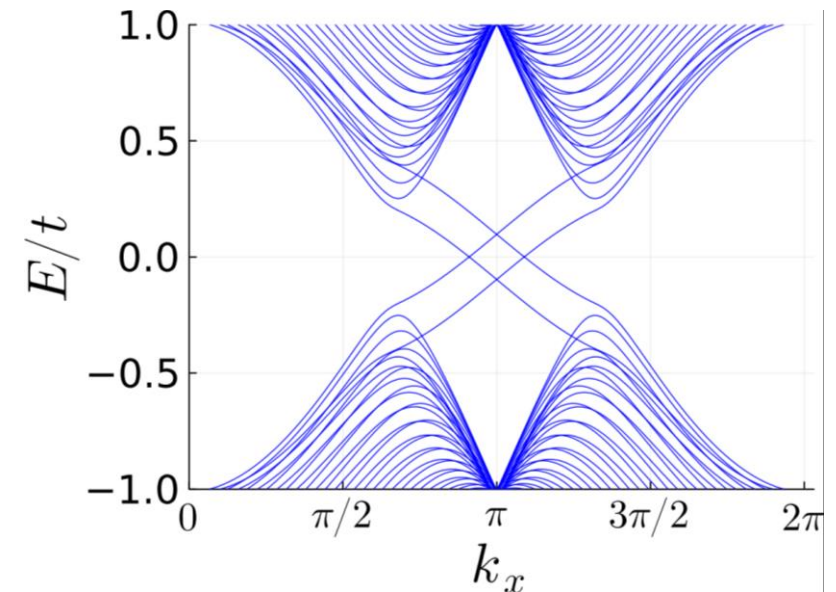
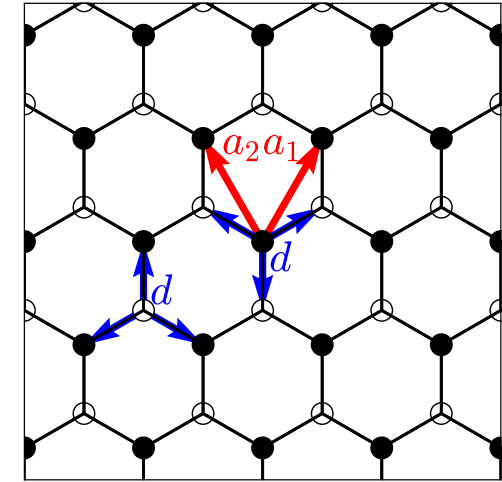
My previous study : Topological Insulator

Kane-Mele model is the first theoretical proposed Topological Insulator (generalized Quantum Spin Hall Insulator)

$$H_{\text{KM}} = t \sum_{\langle i,j \rangle} c_i^\dagger c_j + i\lambda_{\text{SO}} \sum_{\langle\langle i,j \rangle\rangle} \nu_{ij} c_i^\dagger s^z c_j + \lambda_v \sum_i \xi_i c_i^\dagger c_i$$

$$(-1)^\nu = \prod_{i=1}^4 \zeta(\mathbf{\Lambda}_i)$$

$\zeta(\mathbf{\Lambda}_i)$: Parity at time reversal momentum $\mathbf{\Lambda}_i$





My previous study : Bose-Hubbard Model

Calculation was so heavy I could not completely calculate fourth perturbation

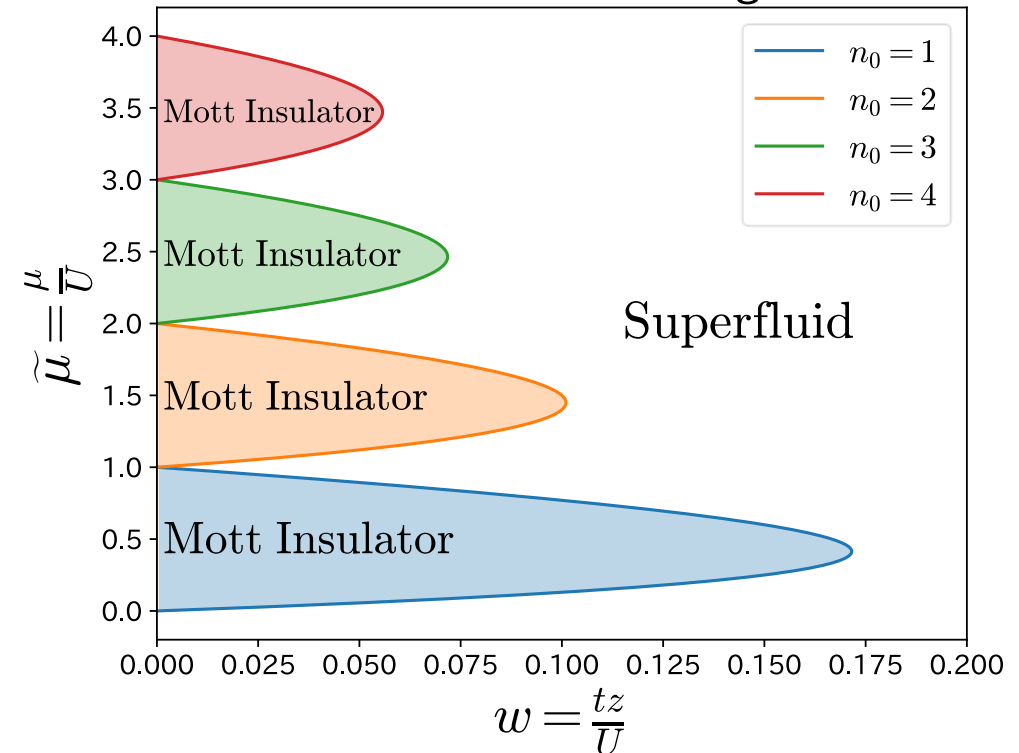
$$H_{\text{BH}} = \sum_{\mathbf{R}} (\epsilon_{\mathbf{R}} - \mu) a_{\mathbf{R}}^{\dagger} a_{\mathbf{R}} - t \sum_{\mathbf{R}} \sum_{i=1}^D (a_{\mathbf{R}}^{\dagger} a_{\mathbf{R}+\mathbf{e}_i} + \text{h.c.}) + \frac{U}{2} \sum_{\mathbf{R}} \hat{n}_{\mathbf{R}} (\hat{n}_{\mathbf{R}} - 1)$$

$$\Xi_{\text{BH}} = \int \mathcal{D}\alpha^* \mathcal{D}\alpha \mathcal{D}\Psi^* \mathcal{D}\Psi \exp[-S_{\text{BH}}[\alpha^*, \alpha, \Psi^*, \Psi]]$$

$$S_{\text{BH}}[\alpha^*, \alpha, \Psi^*, \Psi] = \int_0^{\beta} d\tau \left\{ \sum_{\mathbf{R}} \left(\alpha_{\mathbf{R}}^* (\partial_{\tau} + \epsilon_{\mathbf{R}} - \mu) \alpha_{\mathbf{R}} + \frac{U}{2} \alpha_{\mathbf{R}}^* \alpha_{\mathbf{R}}^* \alpha_{\mathbf{R}} \alpha_{\mathbf{R}} \right) - \sum_{\mathbf{R}} (\alpha_{\mathbf{R}}^* \Psi_{\mathbf{R}} + \Psi_{\mathbf{R}}^* \alpha_{\mathbf{R}}) + \sum_{\mathbf{R}, \mathbf{R}'} \Psi_{\mathbf{R}}^* t_{\mathbf{R}, \mathbf{R}'}^{-1} \Psi_{\mathbf{R}'} \right\} = S_0 + S_{\Psi}$$

$$\begin{cases} S_0 = \int_0^{\beta} d\tau \sum_{\mathbf{R}} \left(\alpha_{\mathbf{R}}^* (\partial_{\tau} + \epsilon_{\mathbf{R}} - \mu) \alpha_{\mathbf{R}} + \frac{U}{2} \alpha_{\mathbf{R}}^* \alpha_{\mathbf{R}}^* \alpha_{\mathbf{R}} \alpha_{\mathbf{R}} \right) \\ S_{\Psi} = \int_0^{\beta} d\tau \left[- \sum_{\mathbf{R}} (\alpha_{\mathbf{R}}^* \Psi_{\mathbf{R}} + \Psi_{\mathbf{R}}^* \alpha_{\mathbf{R}}) + \sum_{\mathbf{R}, \mathbf{R}'} \Psi_{\mathbf{R}}^* t_{\mathbf{R}, \mathbf{R}'}^{-1} \Psi_{\mathbf{R}'} \right] \end{cases}$$

BH Model Phase Diagram



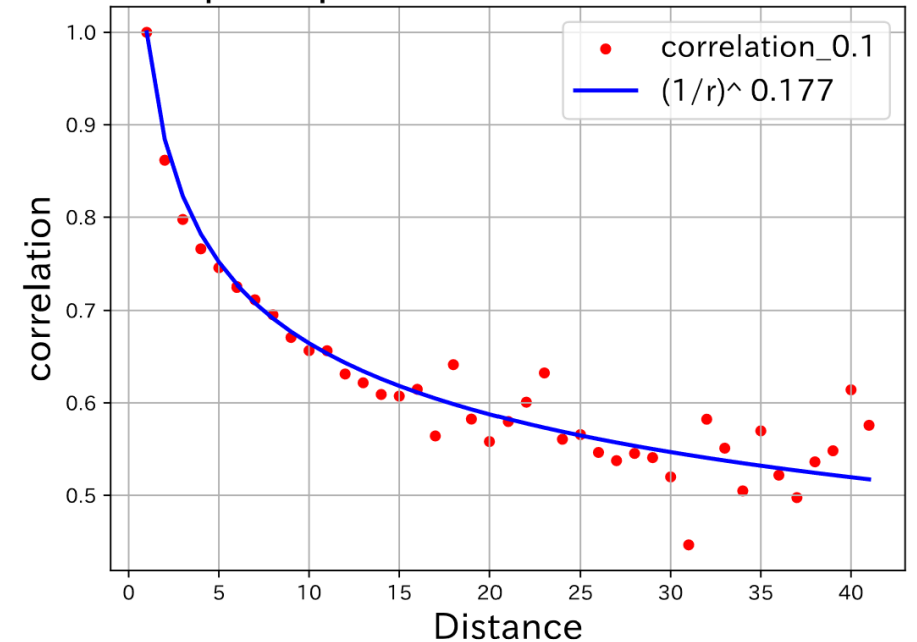
My previous study : Kosterlitz-Thouless transition

$$H_{\text{KT}} = -J \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) = -J \sum_{\langle i,j \rangle} \cos(\theta_i - \theta_j)$$

$$T < T_c : \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \left(\frac{1}{|\mathbf{r}_i - \mathbf{r}_j|} \right)^{-\frac{1}{2\pi J\beta}}$$

$$T > T_c : \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle = \exp\left(-\frac{|\mathbf{r}_i - \mathbf{r}_j|}{\xi}\right), \quad \xi = \left(\log \frac{2}{\beta J}\right)^{-1}$$

Spin-Spin Correlation function



Not good



2. Review of the Topology in Condensed Matter Physics

2.1. What is the topology?

2.2. Topology in Condensed Matter Physics

2.3. Review of Quantum Hall Effect and TKNN formula

2.4. Review of the Topological pump



What is the Topology?

- ✓ “Equivalent” in topology is if and only if two shapes can be **Continuously Deformed** to each other
- ✓ Topological number in this case is a hole that does not change in continuous deformation



Continuously Deform



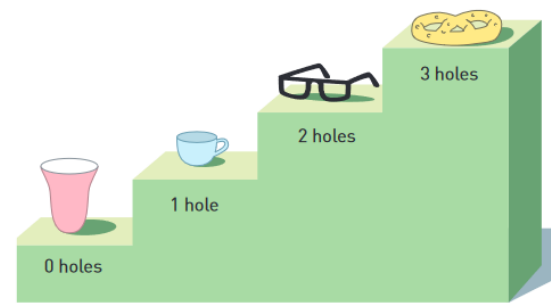
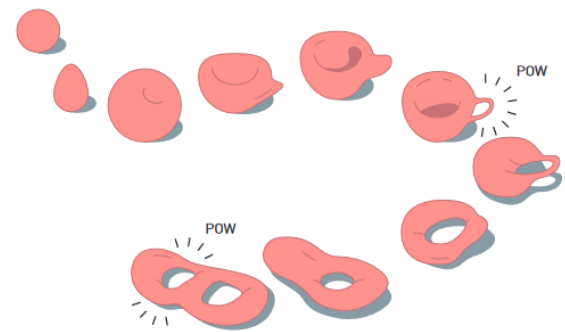


Topology in Condensed Matter Physics



Topology in Condensed Matter Physics
Example : Nobel prize in physic in 2016

- ✓ TKNN Formula
- ✓ Haldane Conjecture
- ✓ Kosterlitz-Thouless transition



© Nobel Media AB. Photo: A. Mahmoud
David J. Thouless
Prize share: 1/2



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Topology in Condensed Matter Physics

Before starting main slides.....

There are a lot of interesting topics in Topological Condensed matter Physics

- Fractional Quantum Hall Effect
- Topological Insulator and Topological Superconductor
- Quantum spin liquid
- Classifications of Topological Phase of Matter (Topological order, SPT, SET...)

See a good review : X. G. Wen, Rev. Mod. Phys. **89**, 041004 (2017)

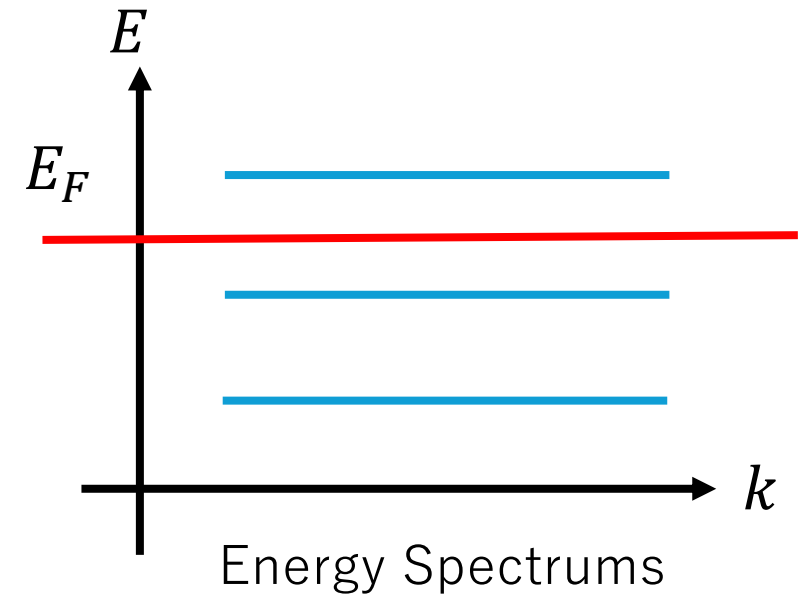
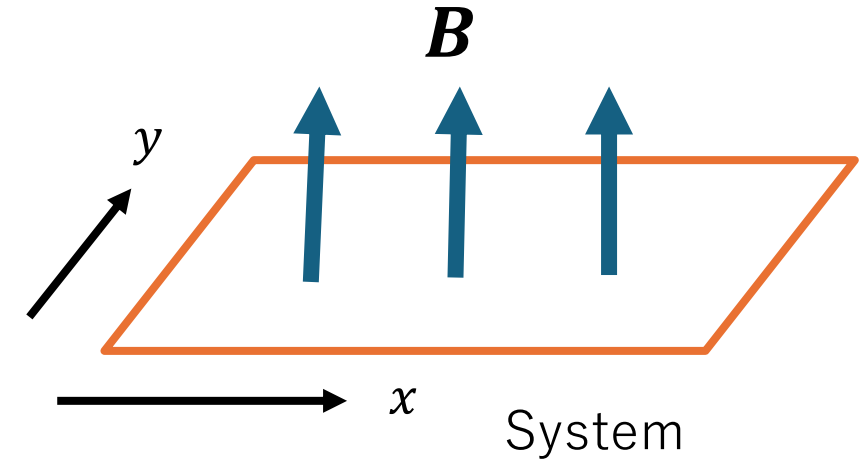
Review of Quantum Hall Effect and TKNN formula

2D system with vertical magnetic field.

Energy eigenvalues are quantized (Landau Level)

Hall conductivity are quantized by integer C
(**Chern Number**)

$$\sigma_{xy} = \frac{e^2}{h} C \quad (j_x = \sigma_{xy} E_y)$$





Review of Quantum Hall Effect and TKNN formula

$$C = \sum_{n=1}^{\text{occ}} C_n = \sum_{n=1}^{\text{occ}} \frac{1}{2\pi} \int_{\text{BZ}} d^2k \mathcal{B}_n(\mathbf{k}) \quad \text{Chern Number}$$

$$\mathcal{B}_n(\mathbf{k}) = \nabla_{\mathbf{k}} \times \mathcal{A}_n(\mathbf{k}) \quad \text{Berry Curvature}$$

$$[\mathcal{A}_n(\mathbf{k})]_i = i \langle u_{n,\mathbf{k}} | \frac{\partial}{\partial k_i} | u_{n,\mathbf{k}} \rangle \quad \text{Berry Connection}$$

The Chern number is Topological number.

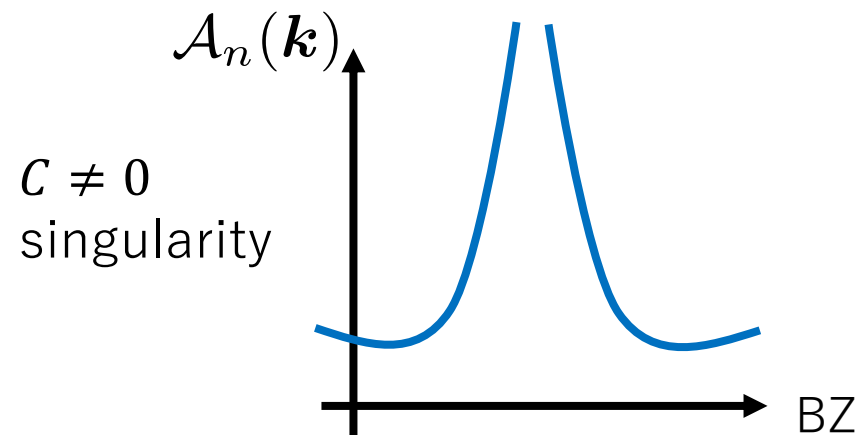
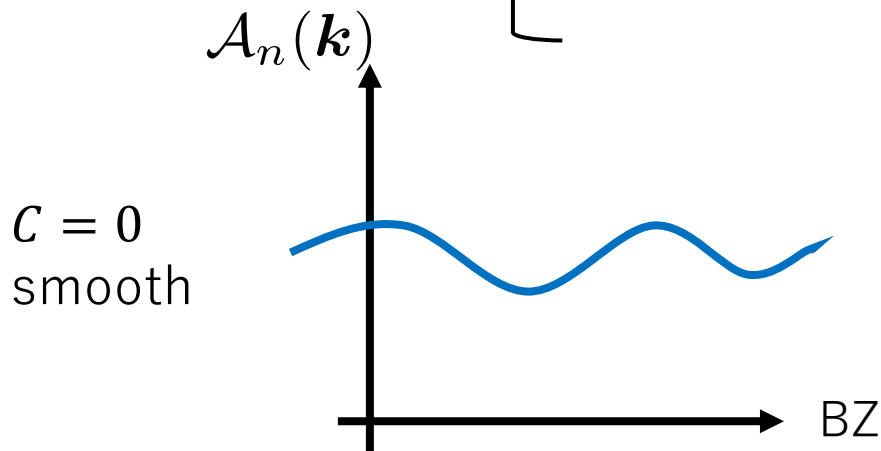
This mathematical formula is called **TKNN formula**

Review of Quantum Hall Effect and TKNN formula

Why Chern Number is topological number? (Physical meaning)

Chern Number corresponds to whether **Berry Connection** $\mathcal{A}_n(\mathbf{k})$ can be smoothly defined or not by one gauge in the BZ.

Chern number = $\left\{ \begin{array}{l} \text{Zero : can be smoothly defined by one gauge} \\ \text{Non-zero: cannot be smoothly defined by one gauge} \end{array} \right.$

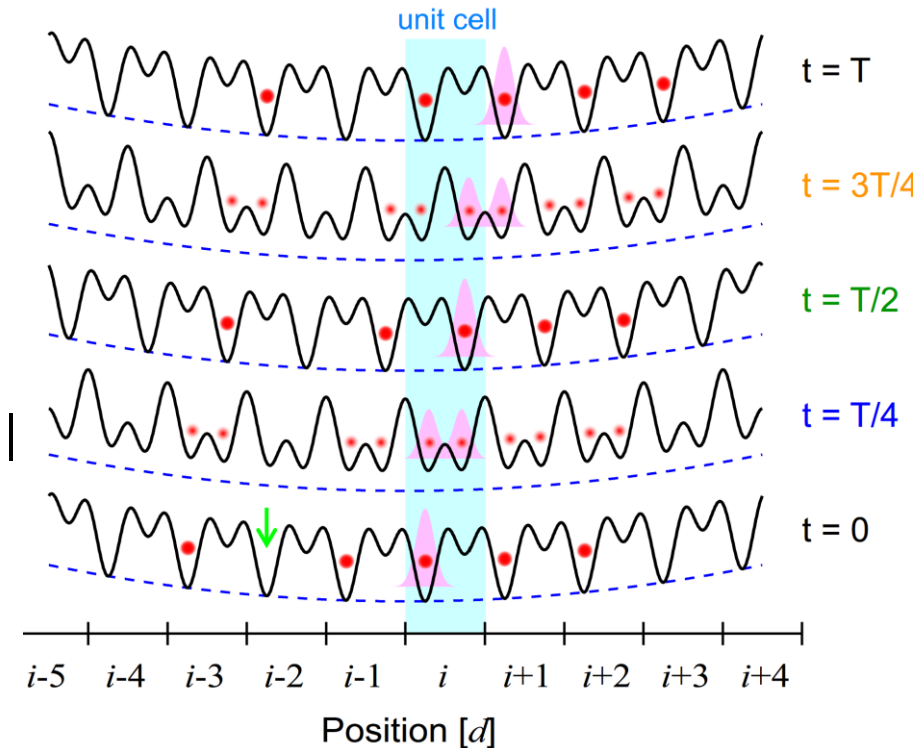




Review of the Topological pump

What is Topological Pump (or Thouless Pump)?

- ✓ We consider 1+1D system and the potential is periodic both in time and space.
- ✓ The charge pumped by the time dependent potential is a topological quantum number.
- ✓ This topological quantum number is Chern number



Nakajima et al., *Nature Phys* **12**, 296–300 (2016)



Review of the Topological pump

We define the Wannier function by Fourier transformation of Bloch wave function.

$$|\mathbf{R}n\rangle = \frac{V}{(2\pi)^3} \int_{\text{BZ}} d^3k e^{-i\mathbf{k}\cdot\mathbf{R}} |\psi_{n,\mathbf{k}}\rangle$$

$|\psi_{n,\mathbf{k}}\rangle$ is the Bloch wave function

Properties:

- ✓ Spans the same Hilbert space that spanned by Bloch wave function
➔ **Contains the same information!**
- ✓ Localized basis
➔ **can be used to construct the Maximally localized basis in real space**
- ✓ Depends on the gauge of Bloch function
➔ **No longer eigenstates of Hamiltonian**



Review of the Topological pump

$$P_\rho(t) = \frac{1}{L} \sum_{n=1}^{\text{occ}} \langle R = 0n, t | \hat{x} | R = 0n, t \rangle$$

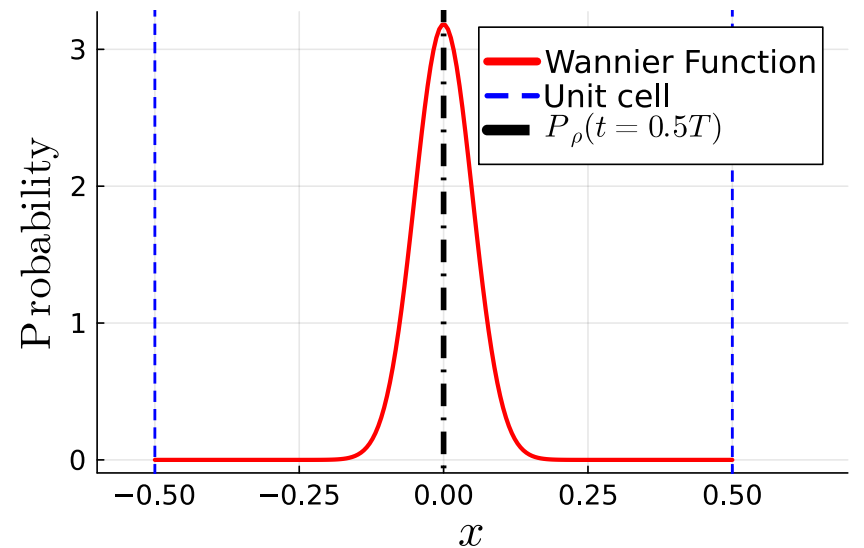
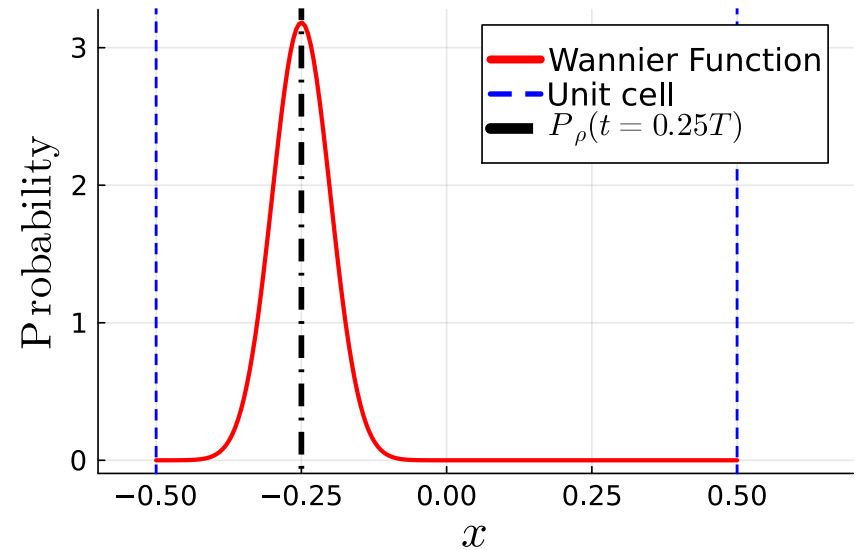
$|Rn, t\rangle$ is Wannier Functions at unit cell R

$$P_\rho(T) - P_\rho(0) = \frac{1}{2\pi} \sum_n^{\text{occ}} \int_0^T dt \int_{-\pi}^{\pi} dk \mathcal{B}_n(k, t)$$

$$\mathcal{B}_n(k, t) = \frac{\partial}{\partial k} [\mathcal{A}_n(k, t)]_t - \frac{\partial}{\partial t} [\mathcal{A}_n(k, t)]_k$$

$$[\mathcal{A}_n(k, t)]_k = i \langle u_{n,k}(t) | \frac{\partial}{\partial k} | u_{n,k}(t) \rangle$$

$$[\mathcal{A}_n(k, t)]_t = i \langle u_{n,k}(t) | \frac{\partial}{\partial t} | u_{n,k}(t) \rangle$$





Review of the Topological pump

Example : Rice-Mele Model

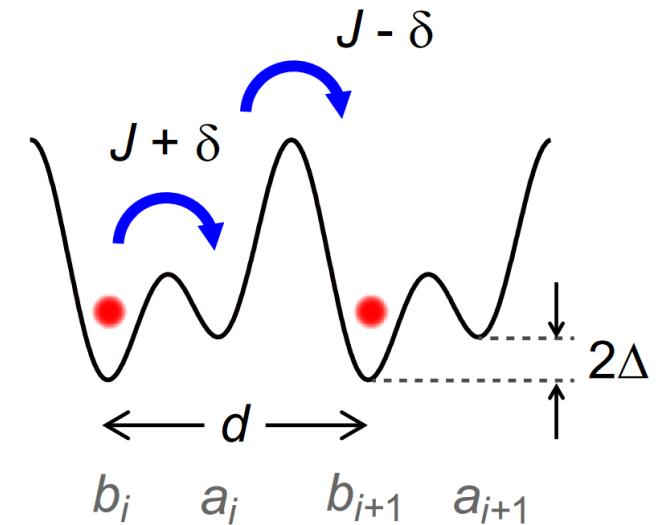
$$\hat{H}_{\text{RM}} = \sum_i \left(-(J + \delta) \hat{a}_i^\dagger \hat{b}_i - (J - \delta) \hat{a}_i^\dagger \hat{b}_{i+1} + \text{h.c.} + \Delta (\hat{a}_i^\dagger \hat{a}_i - \hat{b}_i^\dagger \hat{b}_i) \right)$$

After Fourier transformation, the Hamiltonian is

$$\hat{H}_{\text{RM}} = \sum_k (a_k^\dagger \quad b_k^\dagger) \mathcal{H}(k, t) \begin{pmatrix} a_k \\ b_k \end{pmatrix}$$

$\mathcal{H}(k, t) = \mathbf{R}(k, t) \cdot \boldsymbol{\sigma}$, $\boldsymbol{\sigma}$ is Pauli matrices

$$\mathbf{R}(k, t) = \begin{pmatrix} -2J \cos \frac{kd}{2} \\ 2\delta(t) \sin \frac{kd}{2} \\ \Delta(t) \end{pmatrix}$$



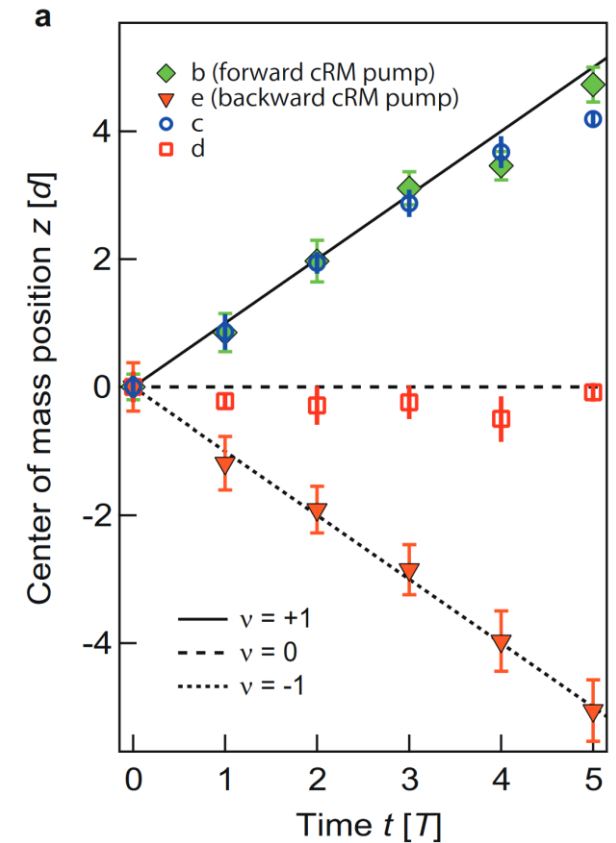
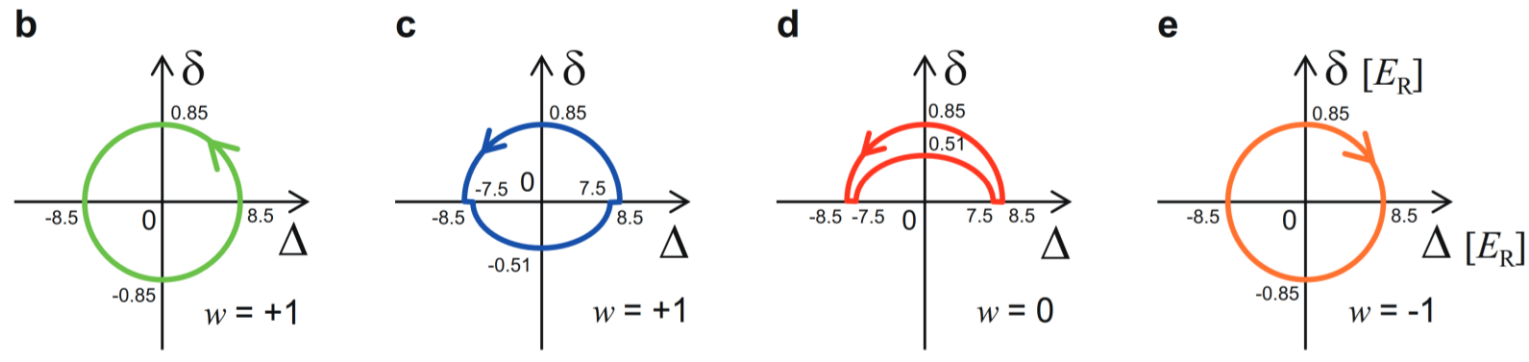
Nakajima et al., *Nature Phys* **12**, 296–300 (2016)



Review of the Topological pump

Example : Rice-Mele Model

After some calculation,
the total charge pumping = the winding number of (Δ, δ) space



Experimentally observed in
Nakajima et al., Nature Phys **12**, 296–300 (2016)



3. Main part : My Research Topic

3.1. *Problem and Motivation*

3.2. *Local Chern Marker*

3.3. *Model*

3.4. *Results*

3.4.1. $\beta = \frac{3}{5}$: *Periodic Case*

3.4.2. $\beta = \frac{2}{\sqrt{5}+1}$: *Non-periodic case*

3.4.3. $\beta = \frac{1}{3}, \frac{2}{3}$: *Domain Wall Case*



Problem and Motivation

- Chern number can only be defined in the quasi-momentum space.
- Chern number assumes that the periodicity of crystal.
- We want to calculate the Chern number without periodicity like quasi-crystal.



Local Chern Marker

We define the Local Chern marker.

$$\mathcal{M}_1(x, t) = \frac{1}{L} \text{Tr}_x [\hat{P}(0) \hat{U}^\dagger(t) \hat{x} \hat{U}(t) \hat{P}(0)]$$

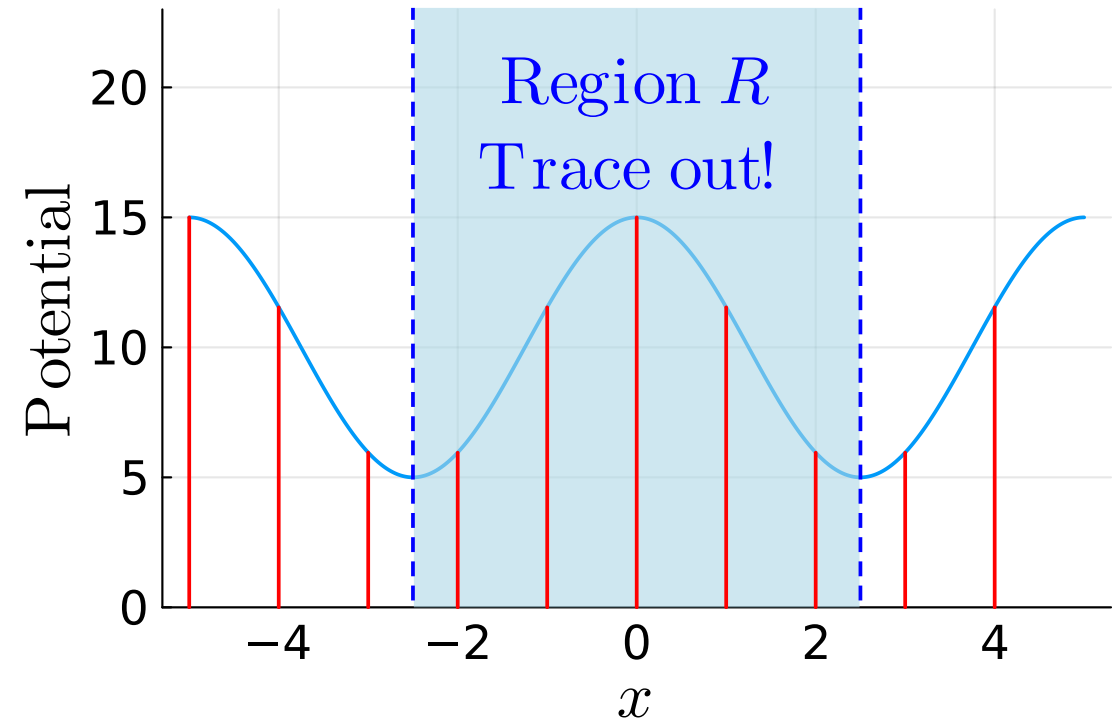
L is the length of the system

$$\text{Tr}_x [\hat{\mathcal{O}}] = \sum_{\alpha} [\langle x | \otimes \langle \alpha |] \hat{\mathcal{O}} [|x\rangle \otimes |\alpha\rangle]$$

α is the internal degrees of freedom

$\hat{P}(t)$ is the projection operator

$\hat{U}(t)$ is the adiabatic time evolution operator



Local Chern Marker at $x = 0$

The region R is 5
Positions within R become
internal degrees of freedom



Local Chern Marker

If **the system has translational invariant (= periodically)**, the difference in one period of the local Chern marker corresponds to the difference in one period of the charge pumping.

$$P_{\rho}(T) - P_{\rho}(0) = \mathcal{M}_1(x, T) - \mathcal{M}_1(x, 0)$$

If the system has translational invariant

Local Chern Marker is the generalization of Chern number in 1+1D!!!



Model

Consider Modulated Kronig-Penney Model with **Open Boundary Condition**.

$$H = -\frac{d^2}{dx^2} + \sum_{j \in \text{system}} h_j^{\alpha\beta\gamma\Delta} \delta(x - x_j^\Delta)$$

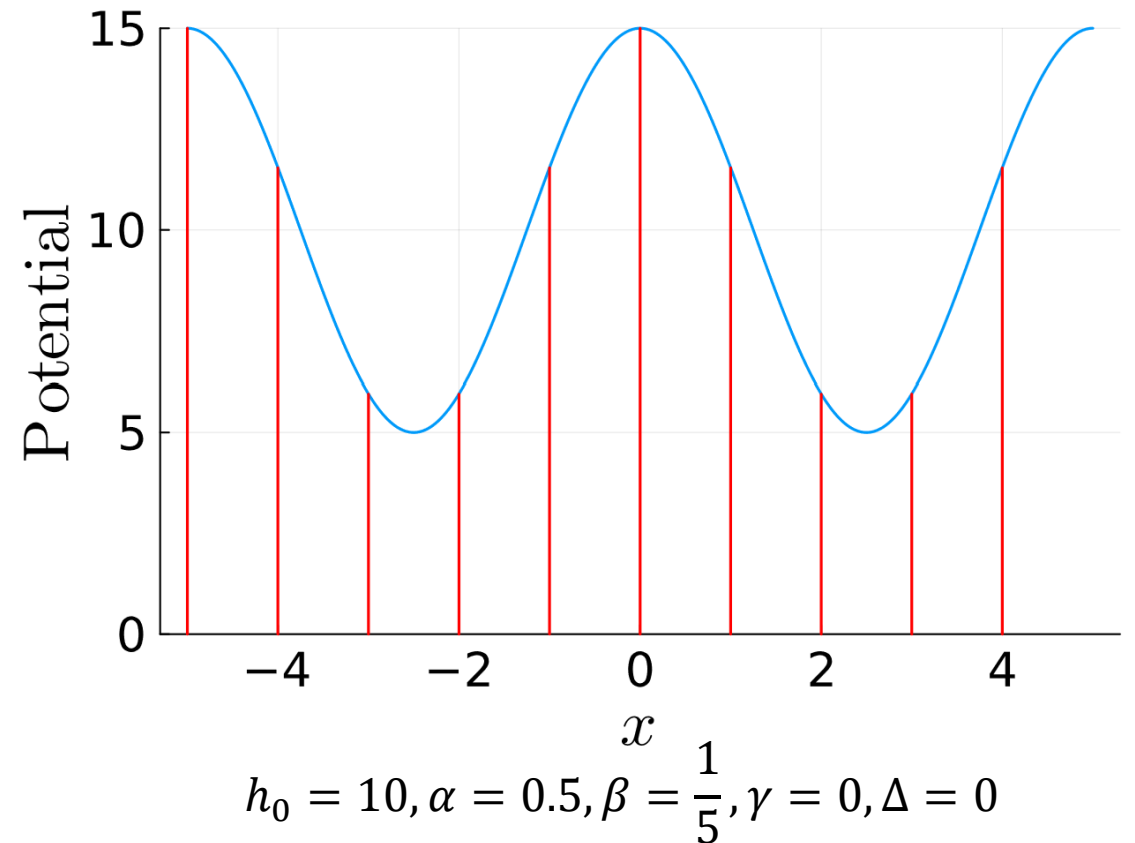
$$h_j^{\alpha\beta\gamma\Delta} = h_0(1 + \alpha \cos(2\pi\beta x_j^\Delta + \gamma))$$

$$x_j^\Delta = x_j + \Delta$$

✓ 1+1D model

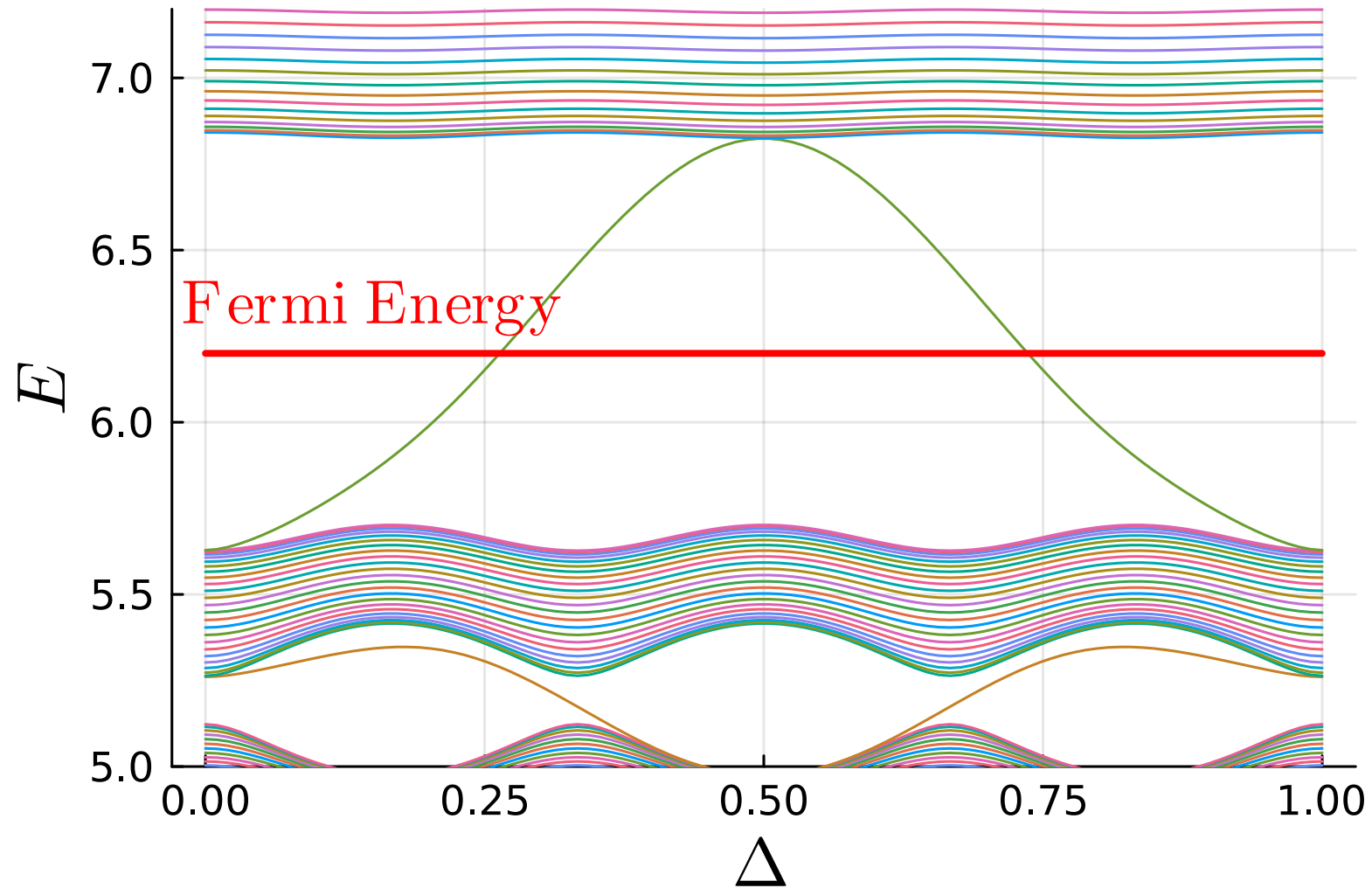
✓ $\Delta \rightarrow t$

✓ Period $T = 1$



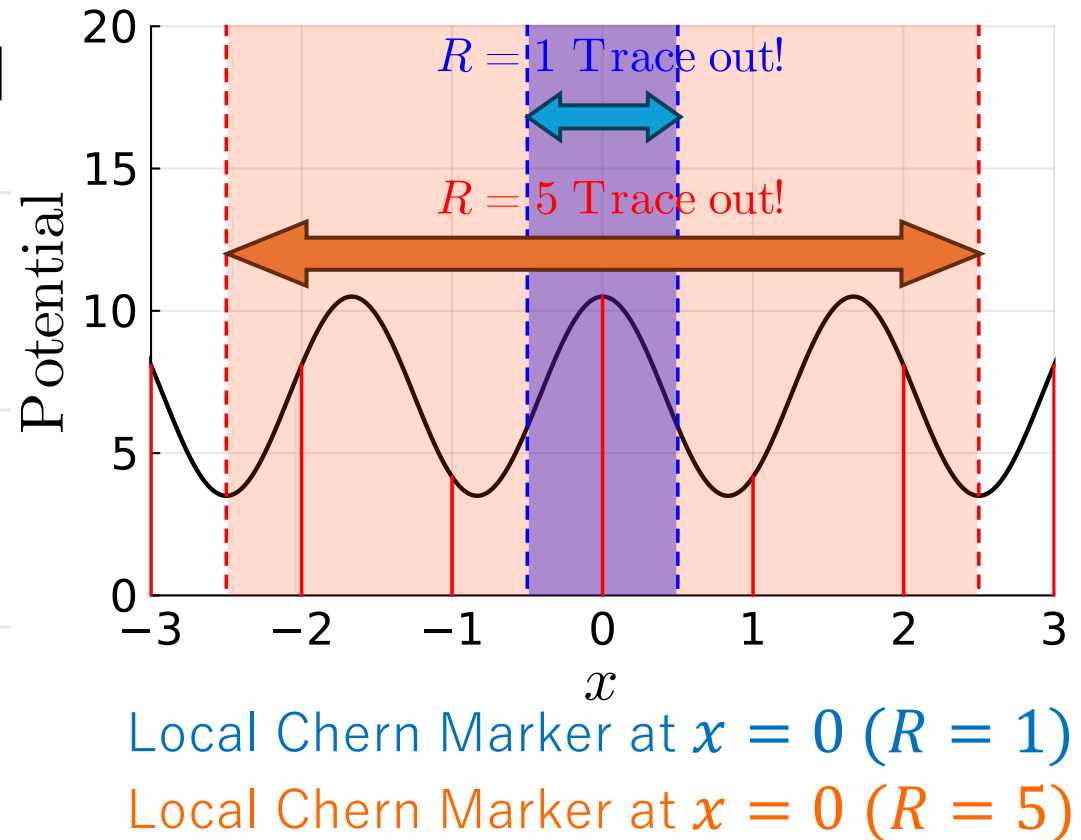
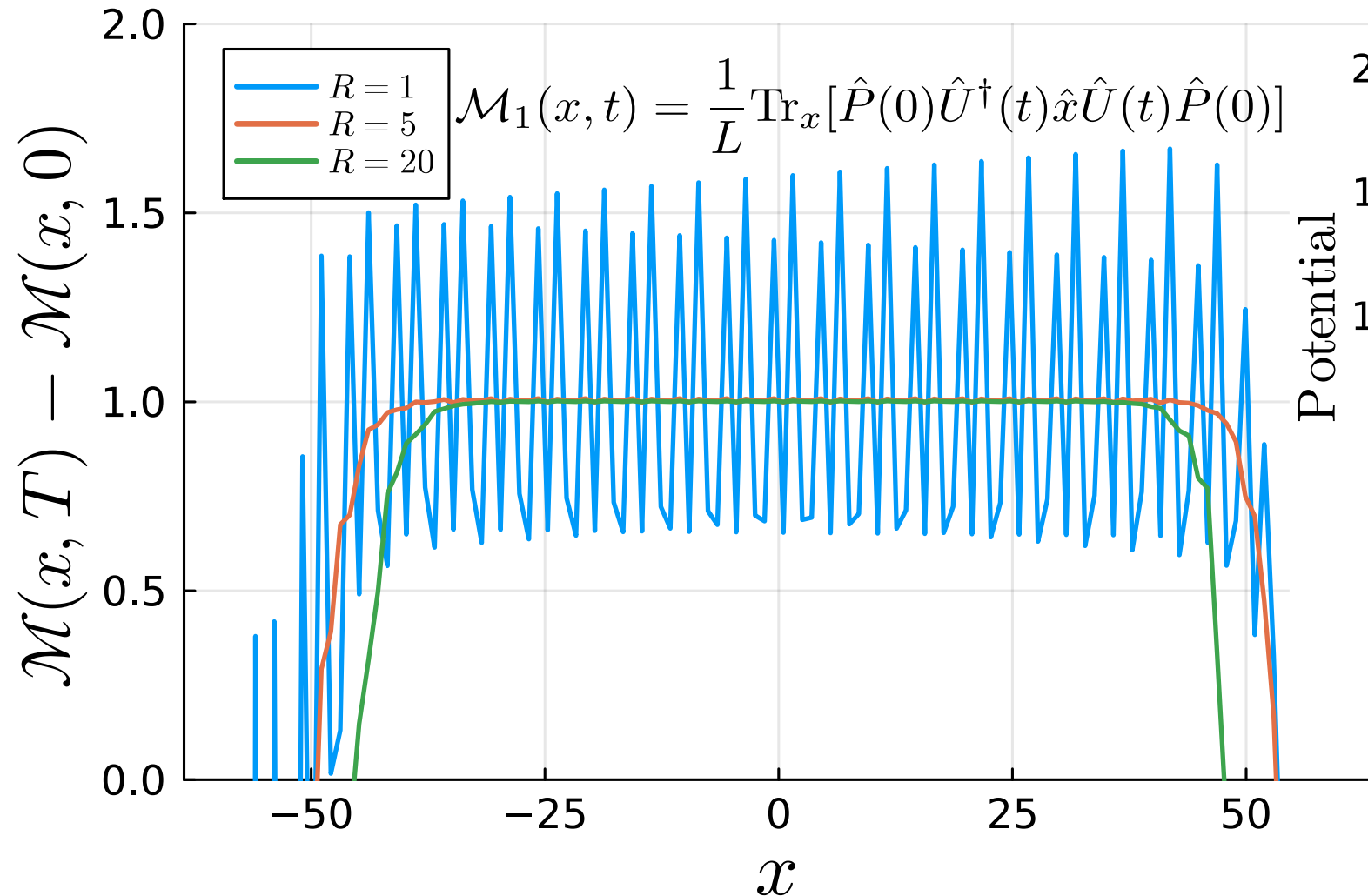


Results of $\beta = \frac{3}{5}$: Periodic Case



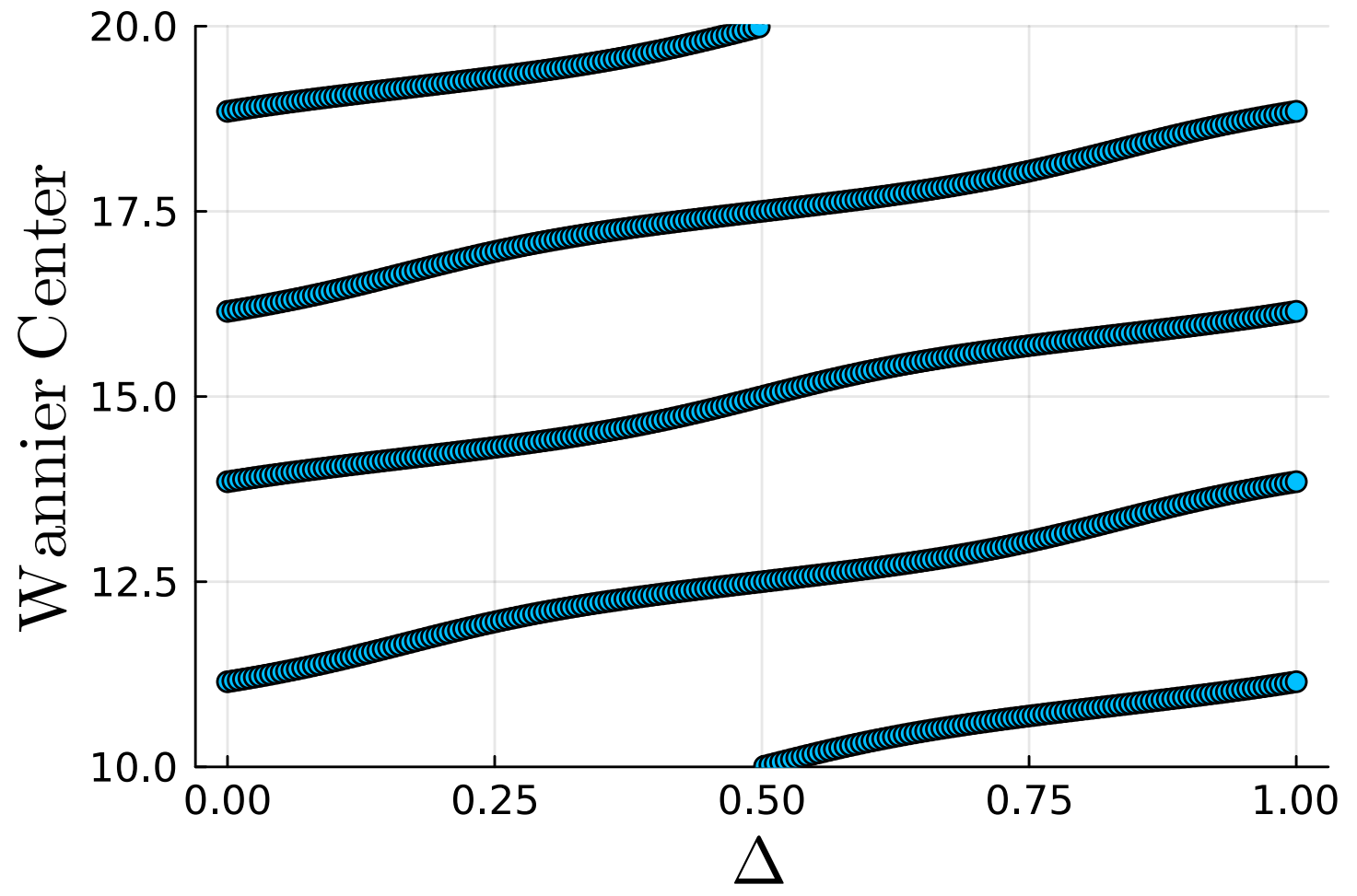


Results of $\beta = \frac{3}{5}$: Periodic Case



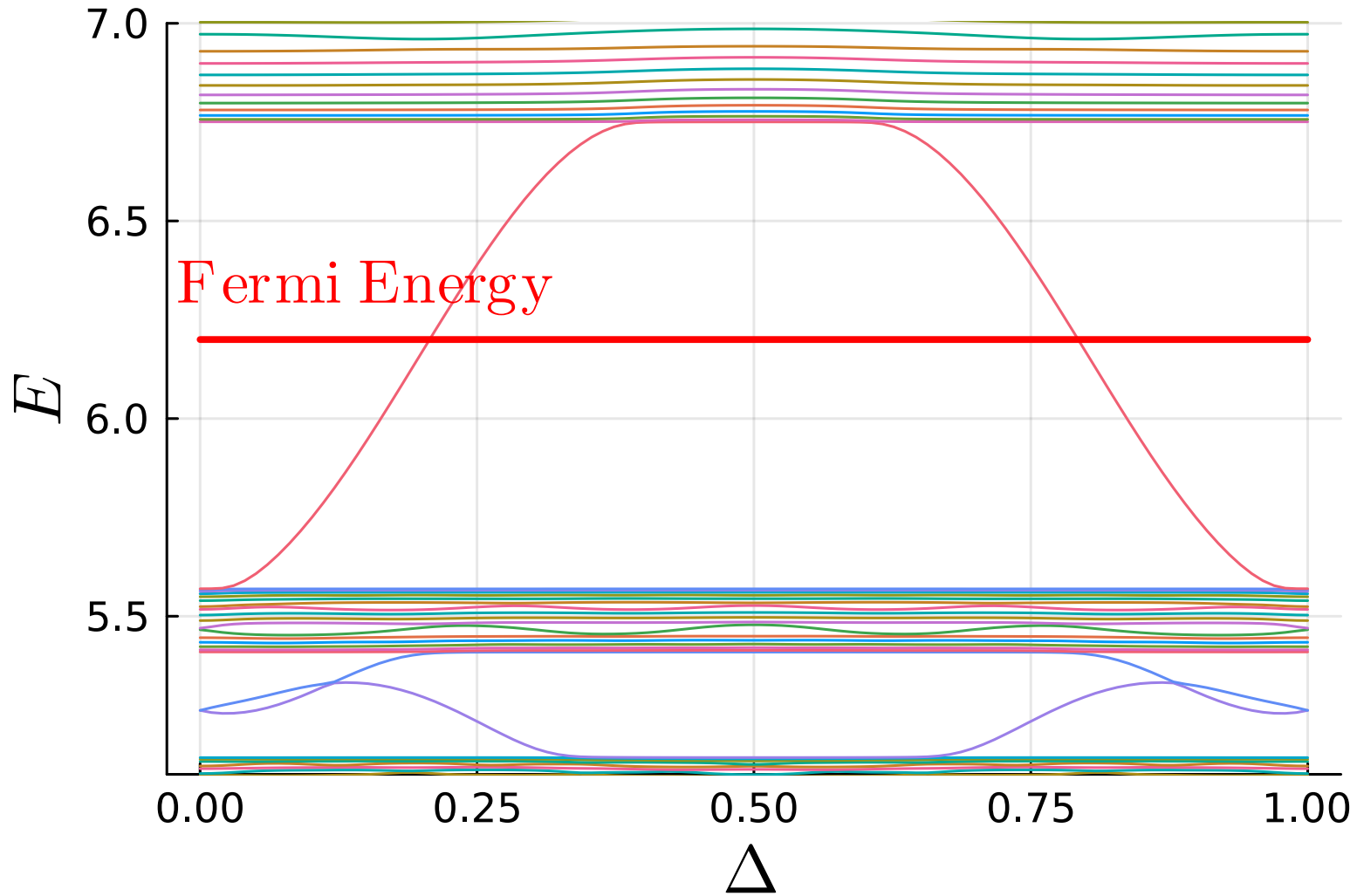


Results of $\beta = \frac{3}{5}$: Periodic Case



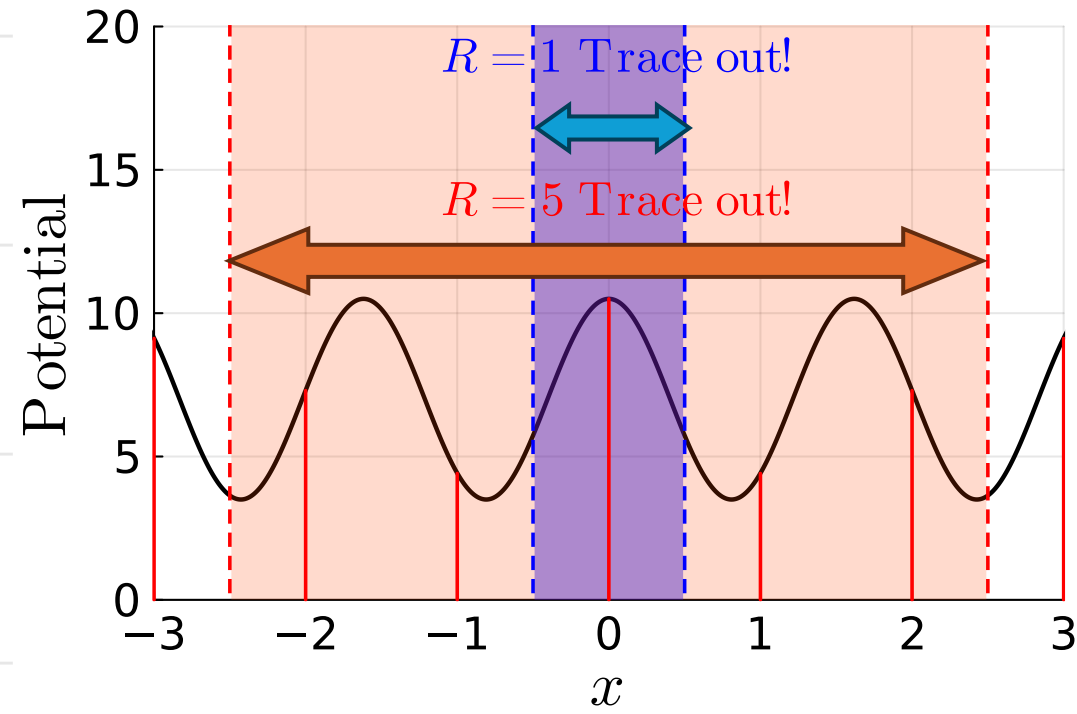
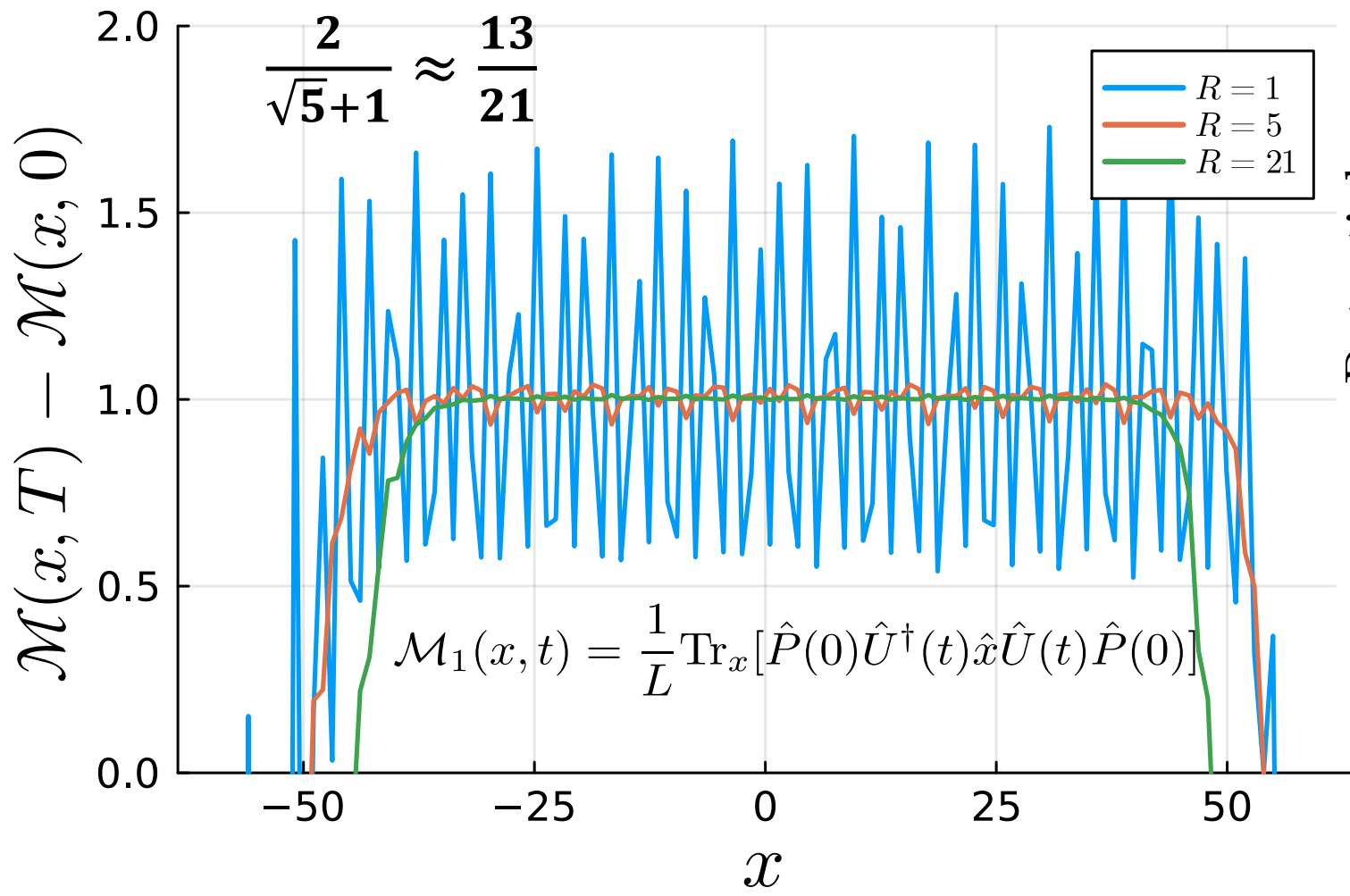


Results of $\beta = \frac{2}{\sqrt{5}+1}$: Non-periodic case





Results of $\beta = \frac{2}{\sqrt{5}+1}$: Non-periodic case

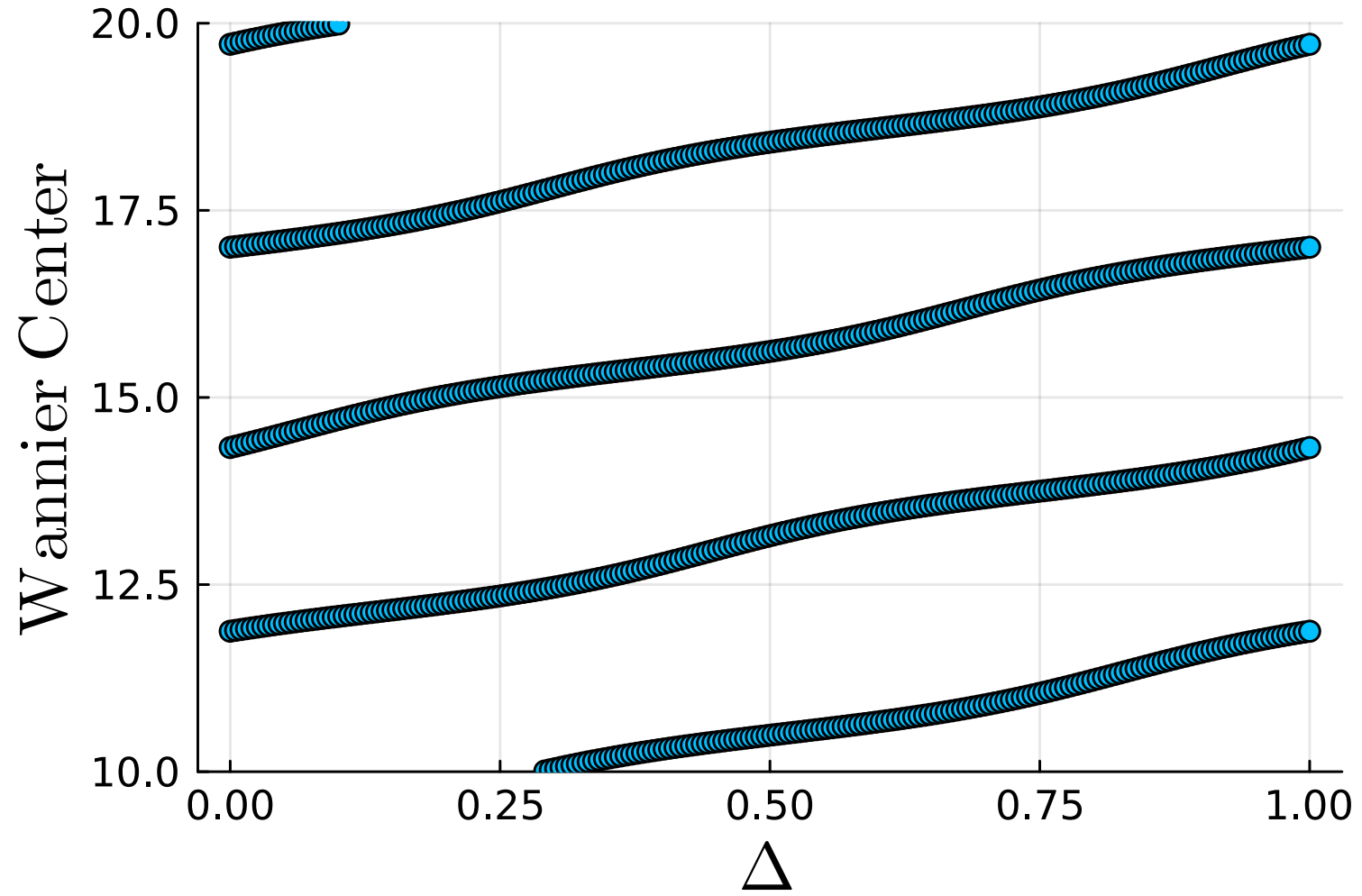


Local Chern Marker at $x = 0$ ($R = 1$)

Local Chern Marker at $x = 0$ ($R = 5$)

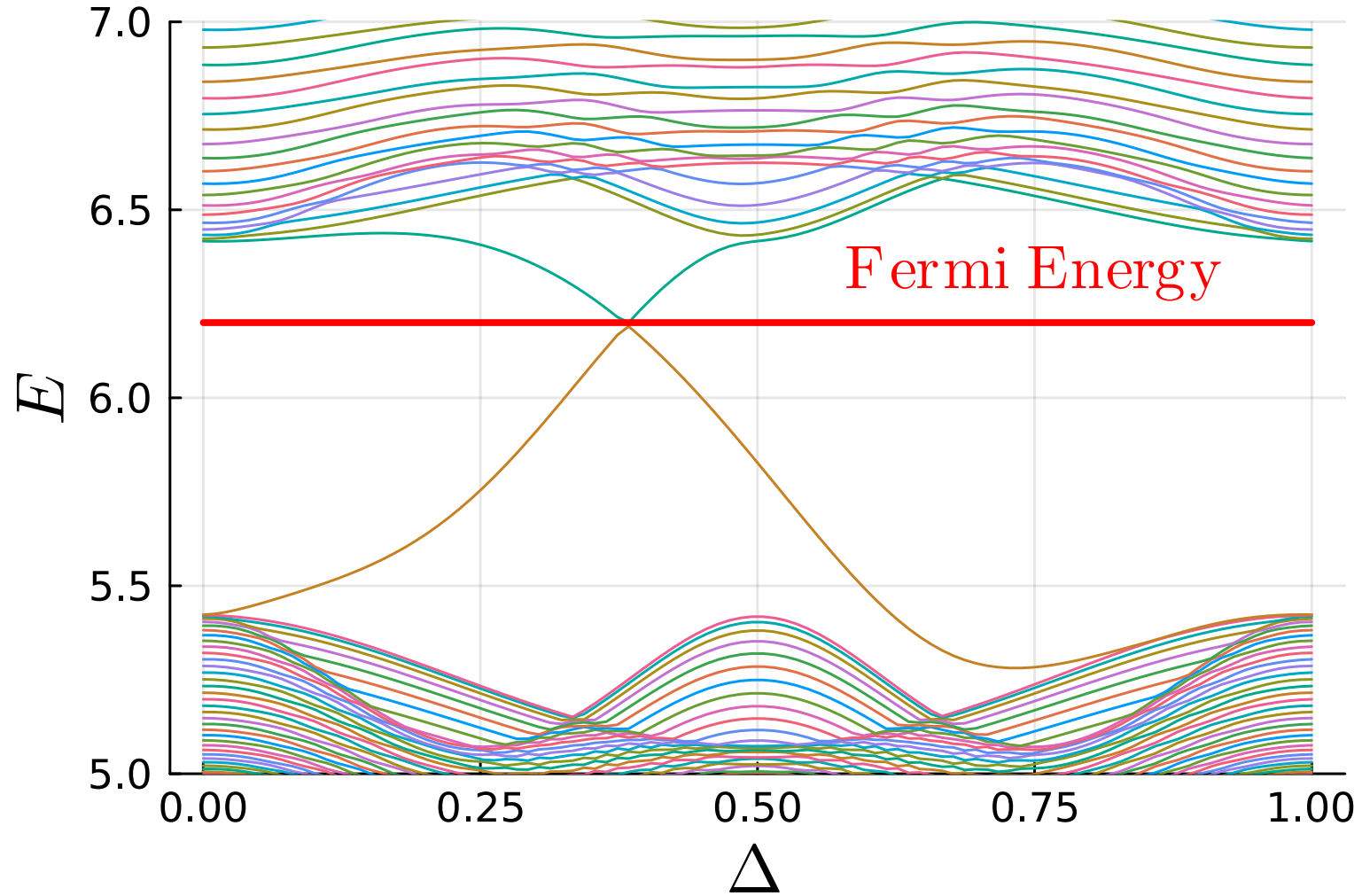


Results of $\beta = \frac{2}{\sqrt{5}+1}$: Non-periodic case



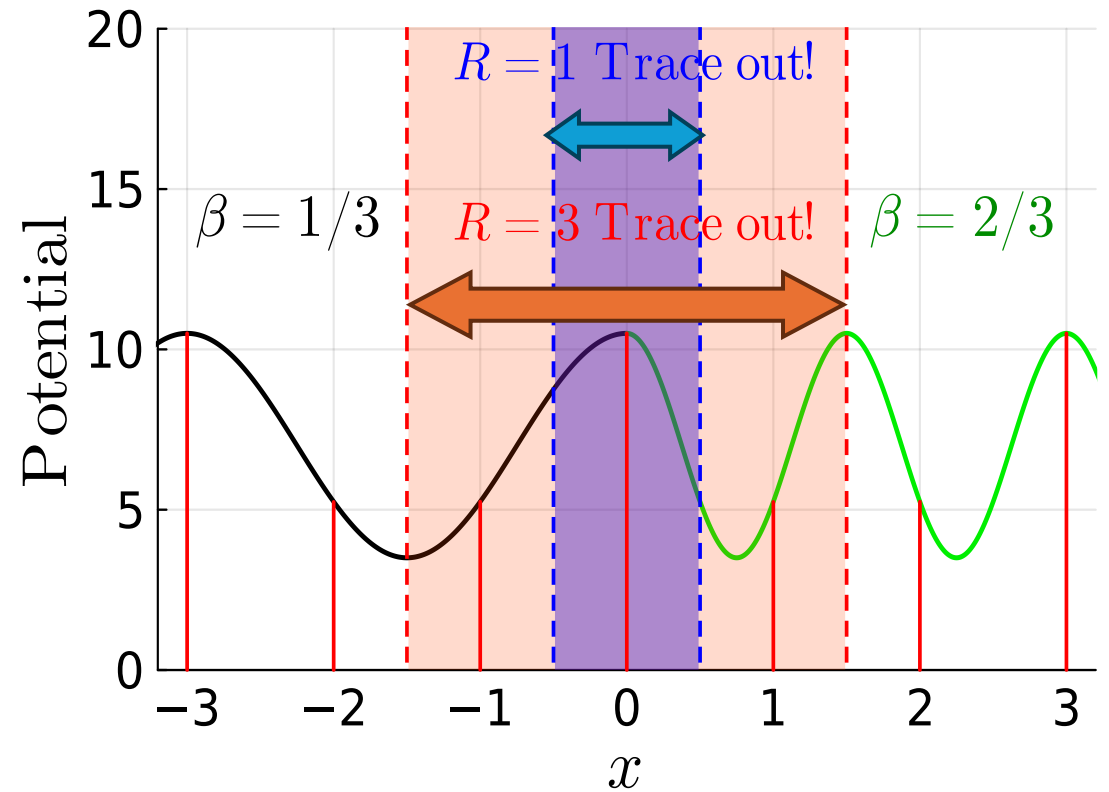
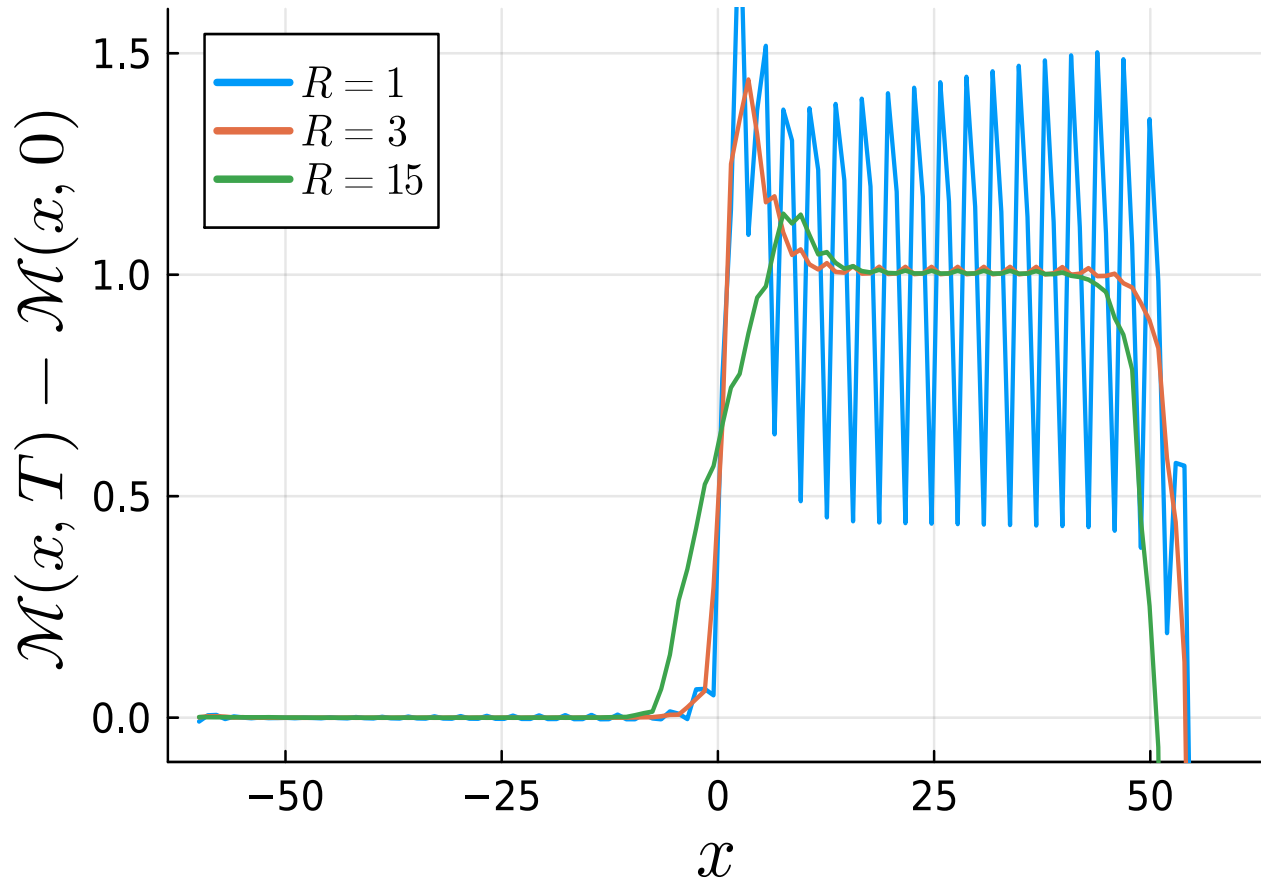


Results of $\beta = \frac{1}{3}, \frac{2}{3}$: Domain Wall Case



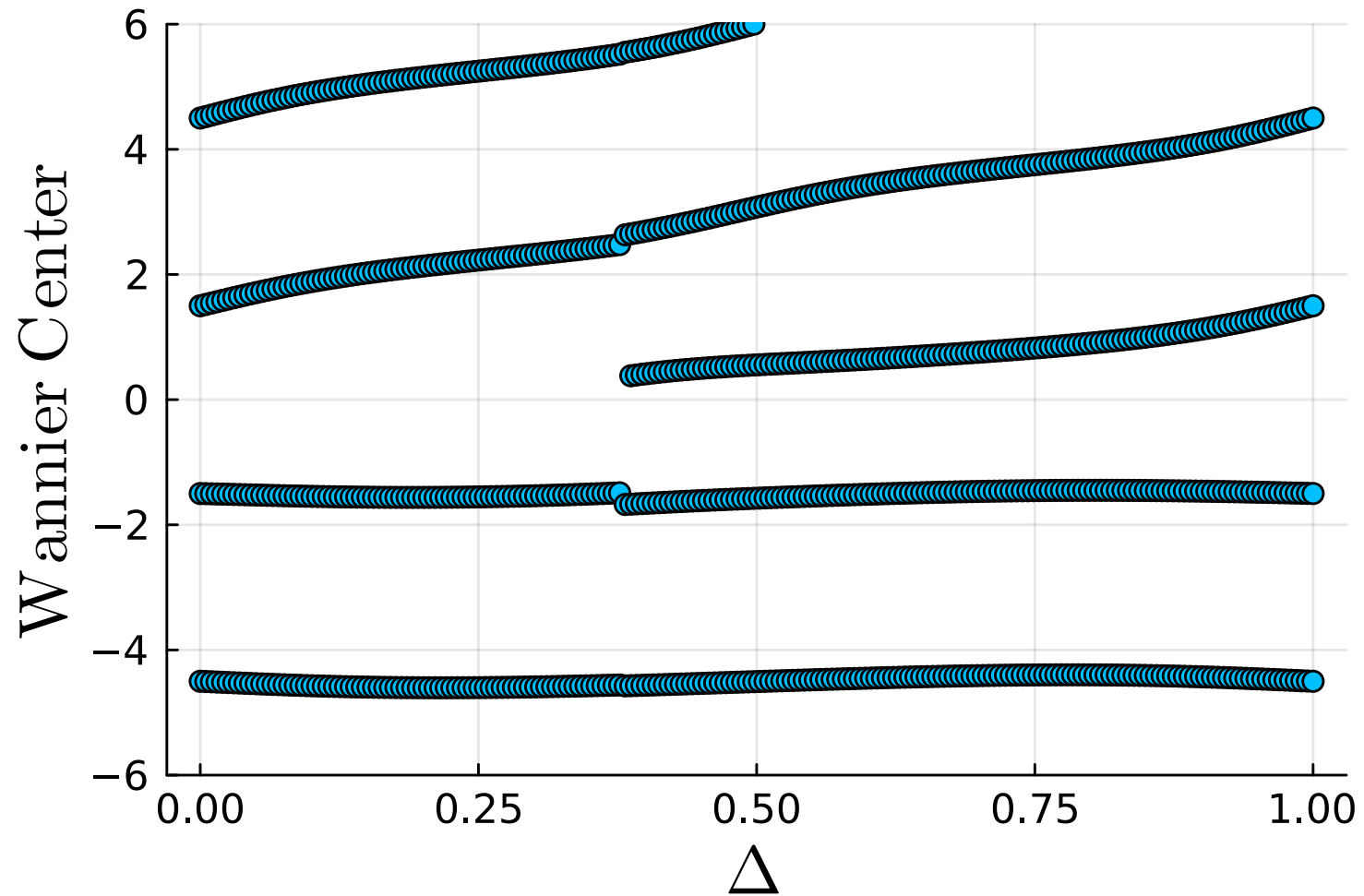


Results of $\beta = \frac{1}{3}, \frac{2}{3}$: Domain Wall Case





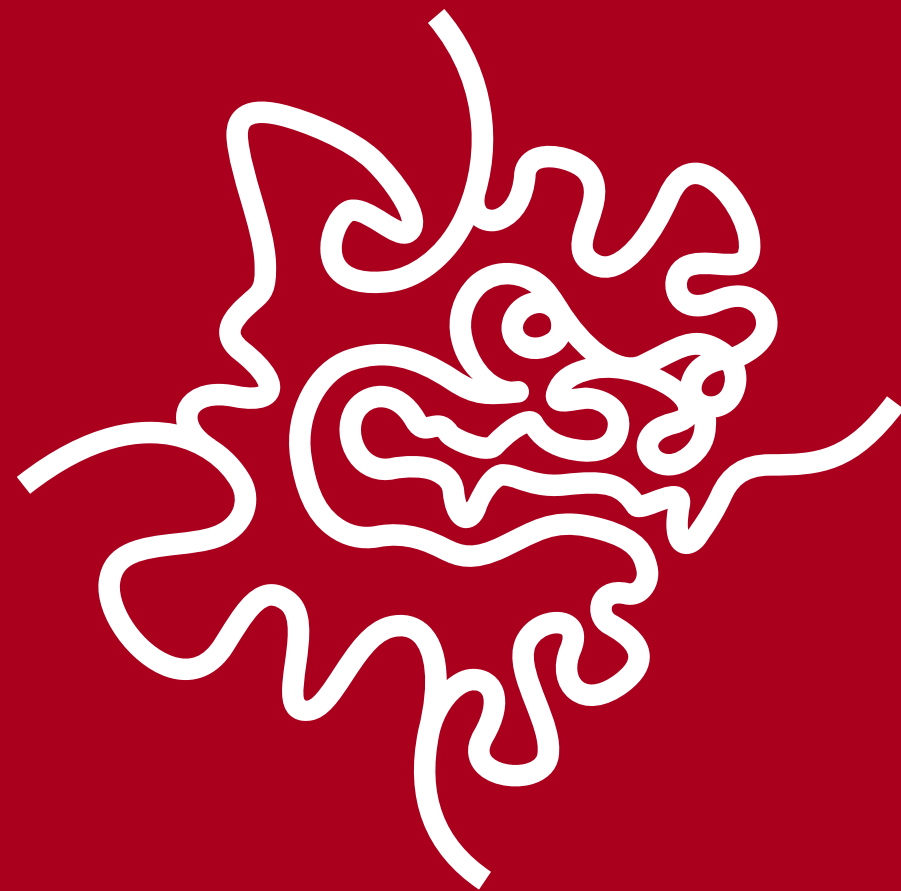
Results of $\beta = \frac{1}{3}, \frac{2}{3}$: Domain Wall Case





Acknowledgment





Thank you!
ありがとうございました！