Note on Chern number

Ning Sun

(Dated: September 27, 2016)

Contents

I. CHERN NUMBER DISCRETIZED

Follow the method that Fukui et.al. has developed in [1], we summarize here the simple way to calculate Chern number numerically in discretized parameter space.

a. Several things to be noticed:

- We restrict our discussion within physical systems of periodical lattice (or what like a periodical lattice) which could be well understood under the band theory frame.
- We point out here that this method is essentially a process of construction of Wilson loop at each plaquette of the discretized parameter space (mostly, torus).
- This method avoid of a procedure of smoothing gauge, an advantage based on merit of last point, that is Wilson loop is gauge-independent.

b. 1st Chern class Here we restrict our discussion within 2-dimensional cases, i.e. the 1st Chern number are we to calculate.

Chern number is defined as

$$c_n = \frac{1}{4\pi}\iint d^2\boldsymbol{k}(\partial_{k_1}\hat{n}\times\partial_{k_2}\hat{n})\cdot\hat{n} \tag{1}$$

where the direction vector $\hat{n}$ is as a function of 2d parameter $\boldsymbol{k}$, i.e. $\hat{n} = \hat{n}(\boldsymbol{k}) = \hat{n}(k_1, k_2)$. And $\hat{n}$ characterize, for a physical system, the direction of the underlying state varying with parameters (k_1, k_2). For example, $\hat{n} = h(\boldsymbol{q})/|h(\boldsymbol{q})|$ with $h(\boldsymbol{q})$ the parametrized Hamiltonian in $\boldsymbol{q}-$space for a two-level system when we consider the Chern number of the upper band.

For a lattice system with $|n(\boldsymbol{k})\rangle$ as its periodic Bloch wave-function of nth band, we define Berry connection and Berry curvature as

$$\begin{aligned}\mathcal{A}_\mu^{(n)} &= \mathrm{i}\langle n(\boldsymbol{k})|\partial_\mu n(\boldsymbol{k})\rangle \\ \mathcal{F}_{\mu\nu}^{(n)} &= \partial_\mu\mathcal{A}_\nu - \partial_\nu\mathcal{A}_\mu \\ &= \mathrm{i}\Big[\langle\partial_\mu n(\boldsymbol{k})|\partial_\nu n(\boldsymbol{k})\rangle - \langle\partial_\nu n(\boldsymbol{k})|\partial_\mu n(\boldsymbol{k})\rangle\Big]\end{aligned}$$

Then we introduce the 1st Chern number to characterize the integral of Berry field defined on a torus $k_x \times k_y$ as

$$\begin{aligned} c_n &= \frac{1}{2\pi} \iint d^2\boldsymbol{k} \mathcal{F}_{xy}^{(n)}(\boldsymbol{k}) \\ &= \frac{1}{2\pi} \iint d^2\boldsymbol{k}\, \mathrm{i} \Big[\langle \partial_x n(\boldsymbol{k}) | \partial_y n(\boldsymbol{k}) \rangle - \langle \partial_y n(\boldsymbol{k}) | \partial_x n(\boldsymbol{k}) \rangle \Big] \end{aligned}$$

c. Numerical procedures

1. Discretize parameter space. Always, it's a torus, by which we mean there are two independent parameters, denoted as k_x, k_y, varying along $0 < k_x \leq 1, 0 < k_y \leq 1$, and we identify each pair of two sides (left and right, top and bottom).
   Also could be other boundary values, not necessary $(0, 1]$, as long as we keep each pair of sides identified.
   Discretizing the parameter torus we get a set of $N \times N$ points each with a coordinate (x_i, y_j). N is the total number of one dimension of the parameter space divided into plaquette.

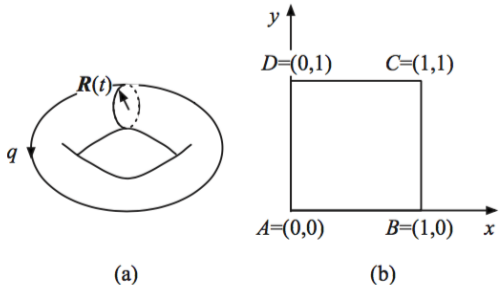
   

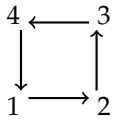
   FIG. 1: Schematic torus topology, from [2]

   We call it (specifically, this set) the *discretized parameter space*.

2. Diagonalizing Hamiltonian $\mathcal{H}(\boldsymbol{k})$ at each single points $\boldsymbol{k} = (x_i, y_j)$ of the discretized parameter space, to obtain a set of eigenvalues $\{\mathcal{E}_n(\boldsymbol{k})\}$ and corresponding eigenvectors $\{|n(\boldsymbol{k})\rangle\}$. n is the band index.

   Again, we require no gauge smoothing procedure, which means that at each parameter point $\boldsymbol{k} = (x_i, y_j)$ there has been chosen an arbitrary gauge for the wave function $\{|n(\boldsymbol{k})\rangle\}$ given by computer program that it could be quite not smooth for two near parameter points $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$, i.e. the wave functions at $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$ might differs a lot. While this results in some singularity in calculating $\mathcal{A}(\boldsymbol{k})$ using numerically differentiation method, it does not affect the calculation of Berry field $\mathcal{F}(\boldsymbol{k})$ as well as its integral the Chern number c_n. This attibutes to the gauge-independency of Wilson loop, which would be seen in later steps.

3. For each parameter point in the discretized parameter space we have obtained in the first step, we construct a Wilson loop around the plaquette locates at this point.

   In numerical calculation, the loop of a plaquette at parameter point $\boldsymbol{k} = (x_i, y_j)$ is chosen as

   $$(x_i, y_j) \to (x_{i+1}, y_j) \to (x_{i+1}, y_{j+1}) \to (x_i, y_{j+1}) \to (x_i, y_j)$$

   with

   $$\begin{aligned} i &= 1, 2, 3, \ldots, N-1 \\ j &= 1, 2, 3, \ldots, N-1 \end{aligned}$$

   Note that the choice might be somewhat "unsymmetrical" in calculating the Berry field strength due to discretization of parameter space. But this would not make big difference in calculation of Chern number as long as we discretize it enough and also makes good approximation to the Berry field (curvature) strength at all points of parameter space.

4. Define for each plaquette

$$U_{12} = V^\dagger(\boldsymbol{k}_2)V(\boldsymbol{k}_1)$$
$$U_{23} = V^\dagger(\boldsymbol{k}_3)V(\boldsymbol{k}_2)$$
$$U_{34} = V^\dagger(\boldsymbol{k}_4)V(\boldsymbol{k}_3)$$
$$U_{41} = V^\dagger(\boldsymbol{k}_1)V(\boldsymbol{k}_4)$$

where $V(\boldsymbol{k})$ is the unitary matrix diagonalizing Hamiltonian at $\boldsymbol{k}$, i.e. the row vector of $V(\boldsymbol{k})$ is normalized eigenvectors of $\mathcal{H}(\boldsymbol{k})$,

$$V^\dagger(\boldsymbol{k})\mathcal{H}(\boldsymbol{k})V(\boldsymbol{k}) = D(\boldsymbol{k})$$

Extract diagonal elements of each link operator U_{ij}, that is, define new link quantity as

$$\mathcal{U}_{ij} = diag(U_{ij})$$

where $diag()$ means to retain all diagonal elements of a matrix while abandon all off-diagonal elements. Easy to see that $\mathcal{U}_{ij}$ are all diagonal matrices. And $\mathcal{U}_{ij}^{mn} = \delta_{mn}U_{ij}^{nn}$.

Define at each $\boldsymbol{k} = (x_i, y_j)$

$$T_{\text{loop}}(\boldsymbol{k}) = \mathcal{U}_{41}\mathcal{U}_{34}\mathcal{U}_{23}\mathcal{U}_{12}$$

The Chern number for nth band is calculated through

$$c_n = \frac{1}{2\pi}\sum_{i=1}^{N-1}\sum_{j=1}^{N-1} -\mathrm{i}\log T_{\text{loop}}^{(nn)}(x_i, y_j) \tag{2}$$

i.e. sum over the angle of the nth diagonal element of $T_{\text{loop}}(\boldsymbol{k})$ at all $\boldsymbol{k} = (x_i, y_j)$.

Berry field at each discretized parameter plaquette for the nth band is just

$$\mathcal{F}_{xy}^{(n)}(\boldsymbol{k}) = \theta_n(\boldsymbol{k})/s(\boldsymbol{k})$$

where $\theta_n(\boldsymbol{k})$ is the angle of the nth diagonal element of $T_{\text{loop}}(\boldsymbol{k})$ and $s(\boldsymbol{k})$ is the area for each plaquette.

$$\theta_n(\boldsymbol{k}) = -\mathrm{i}\log T_{\text{loop}}^{(nn)}(x_i, y_j)$$
$$s(\boldsymbol{k}) = \Delta k_x \Delta k_y$$

d. Justification for the method Why this procedure works? Here's my understanding. I pay attention to two aspects, verifiability of both of which justify its validity. They are *equivalence to the original integral* and *gauge independency*.

Equivalence to the original integral Look at Eq.(2), the nth band Chern number is summation over the angle of the nth diagonal element of T_{loop} at all plaquettes. Then what the nth diagonal element of T_{loop} at each

plaquette exactly is? It is actually

$$\begin{aligned} T^{(nn)}_{\text{loop}}(x_i, y_i) &= (\mathcal{U}_{41}\mathcal{U}_{34}\mathcal{U}_{23}\mathcal{U}_{12})_{nn} = \mathcal{U}^{(nn)}_{41}\mathcal{U}^{(nn)}_{34}\mathcal{U}^{(nn)}_{23}\mathcal{U}^{(nn)}_{12} \\ &= \langle n(\boldsymbol{k}_1)|n(\boldsymbol{k}_4)\rangle\langle n(\boldsymbol{k}_4)|n(\boldsymbol{k}_3)\rangle\langle n(\boldsymbol{k}_3)|n(\boldsymbol{k}_2)\rangle\langle n(\boldsymbol{k}_2)|n(\boldsymbol{k}_1)\rangle \end{aligned}$$

But we know $\boldsymbol{k}_1$, $\boldsymbol{k}_2$, $\boldsymbol{k}_3$, $\boldsymbol{k}_4$ is four corners of a plaquette of the discretized parameter space, so that they are nearly next to each other and form a directional loop. Hence the a typical element is evaluated, up to first order, as

$$\begin{aligned} \langle n(\boldsymbol{k}_2)|n(\boldsymbol{k}_1)\rangle &= \langle n(x_{i+1}, y_j)|n(x_i, y_j)\rangle \\ &= (\langle n(x_i, y_j)| + \Delta k_x \langle \partial_x n(x_i, y_j)|)|n(x_i, y_j)\rangle \\ &= 1 + \Delta k_x \langle \partial_x n(x_i, y_j)|n(x_i, y_j)\rangle \\ &= 1 - \Delta k_x \langle n(x_i, y_j)|\partial_x n(x_i, y_j)\rangle \\ &= 1 + \mathrm{i}\int_1^2 \mathcal{A}(x_i, y_j) d\boldsymbol{k}_x \end{aligned}$$

Similarly are other elements. Thus, to first order again, we obtain

$$T^{(nn)}_{\text{loop}}(x_i, y_i) = 1 + \mathrm{i}\oint_{\square} \mathcal{A}(\boldsymbol{k}) \cdot d\boldsymbol{k} = e^{\mathrm{i}\theta(\boldsymbol{k})}$$

and $\theta(\boldsymbol{k})$ is the $\boldsymbol{k} = (x_i, y_j)$ plaquette's contribution to whole Berry curvature integral. Adding all such terms is the Chern number (times 2π). This is guaranteed by Stokes' theorem.

Gauge independency A simple argument is that Chern number c_n is gauge invariant. So what we got is what we want to get, no concern about gauge smoothing.

But such an argument is somewhat tricky. If it just picks up one gauge at one point and another at another, arbitrarily, what happens at all? Is above deriviation valid as well? Let we look at it explicitly. Suppose

$$|n(\boldsymbol{k})\rangle \to e^{\mathrm{i}\chi(\boldsymbol{k})}|n(\boldsymbol{k})\rangle$$

then

$$\begin{aligned} T^{(n)}(\boldsymbol{k}) &= \langle n(1)|n(4)\rangle\langle n(4)|n(3)\rangle\langle n(3)|n(2)\rangle\langle n(2)|n(1)\rangle \\ &\quad \times e^{\mathrm{i}[\chi(1)-\chi(2)+\chi(2)-\chi(3)+\chi(3)-\chi(4)+\chi(4)-\chi(1)]} \\ &= \langle n(1)|n(4)\rangle\langle n(4)|n(3)\rangle\langle n(3)|n(2)\rangle\langle n(2)|n(1)\rangle \end{aligned}$$

Being gauge invariant, this quantity. This is actually the fact that Berry curvature is a gauge independent quantity.

In conclusion, we trust this method gives valid numerical evaluation of the value of Chern number for a gapped band, and this method is of a merit that need not doing gauge smoothing for wave functions.

e. Precision accuracy How valid is this method? Here's some numerical results.

```
In[32]:= NumberForm[c1, 16]
         NumberForm[c2, 16]
Out[32]//NumberForm=
         0.999999999999996
Out[33]//NumberForm=
         -1.000000000000001
```

(a) case in Fig. 3

```
In[61]:= NumberForm[c1, 16]
         NumberForm[c2, 16]
Out[61]//NumberForm=
         -4.864810407253438×10^-16
Out[62]//NumberForm=
         -1.260738261797028×10^-17
```

(b) case in Fig. 5

FIG. 2: Mathematica numerical results of Chern numbers for Rice-Mele model

We see that, the numerical accuracy can reach at a level $\ll 10^{-10}$.

II. TIME-DEPDENDENT RICE-MELE MODEL

Consider a time-dependent Rice-Mele model[2–4]. Hamiltonian writes

$$H(t) = \sum_j -(J+\delta(t))a_j^\dagger b_j - (J-\delta(t))a_{j+1}^\dagger b_j + h.c. + \Delta(t)(a_j^\dagger a_j - b_j^\dagger b_j)$$

Fourier transformed into (crystal) momentum space we obtain a Hamiltonian with parameters (q,t) as

$$\begin{aligned}\mathcal{H}(q,t) &= -2J\cos(\frac{qa}{2})\sigma_x + 2\delta(t)\sin(\frac{qa}{2})\sigma_y + \Delta(t)\sigma_z \\ &= \boldsymbol{h}(q,t)\cdot\boldsymbol{\sigma} \\ &= \begin{pmatrix} \Delta(t) & -2J\cos\frac{qa}{2} - \mathrm{i}2\delta(t)\sin\frac{qa}{2} \\ -2J\cos\frac{qa}{2} + \mathrm{i}2\delta(t)\sin\frac{qa}{2} & -\Delta(t)\end{pmatrix}\end{aligned}$$

The time dependence is holding in $\delta(t)$ and $\Delta(t)$. In general, we set up

$$\begin{aligned}\delta(t) &= \delta_0 + \delta\sin(\omega t) \\ \Delta(t) &= \Delta_0 + \Delta\cos(\omega t)\end{aligned}$$

The degeneracy point is $\delta(t)=0, \Delta(t)=0$ (if there is). Thus the evolution loop could enclose or not enclose the degeneracy point, relying on whether or not this condition could be reached. Specifically, if $-\delta < \delta_0 < \delta$ and $-\Delta < \Delta_0 < \Delta$, the evolution loop then encloses the degeneracy point, else not.

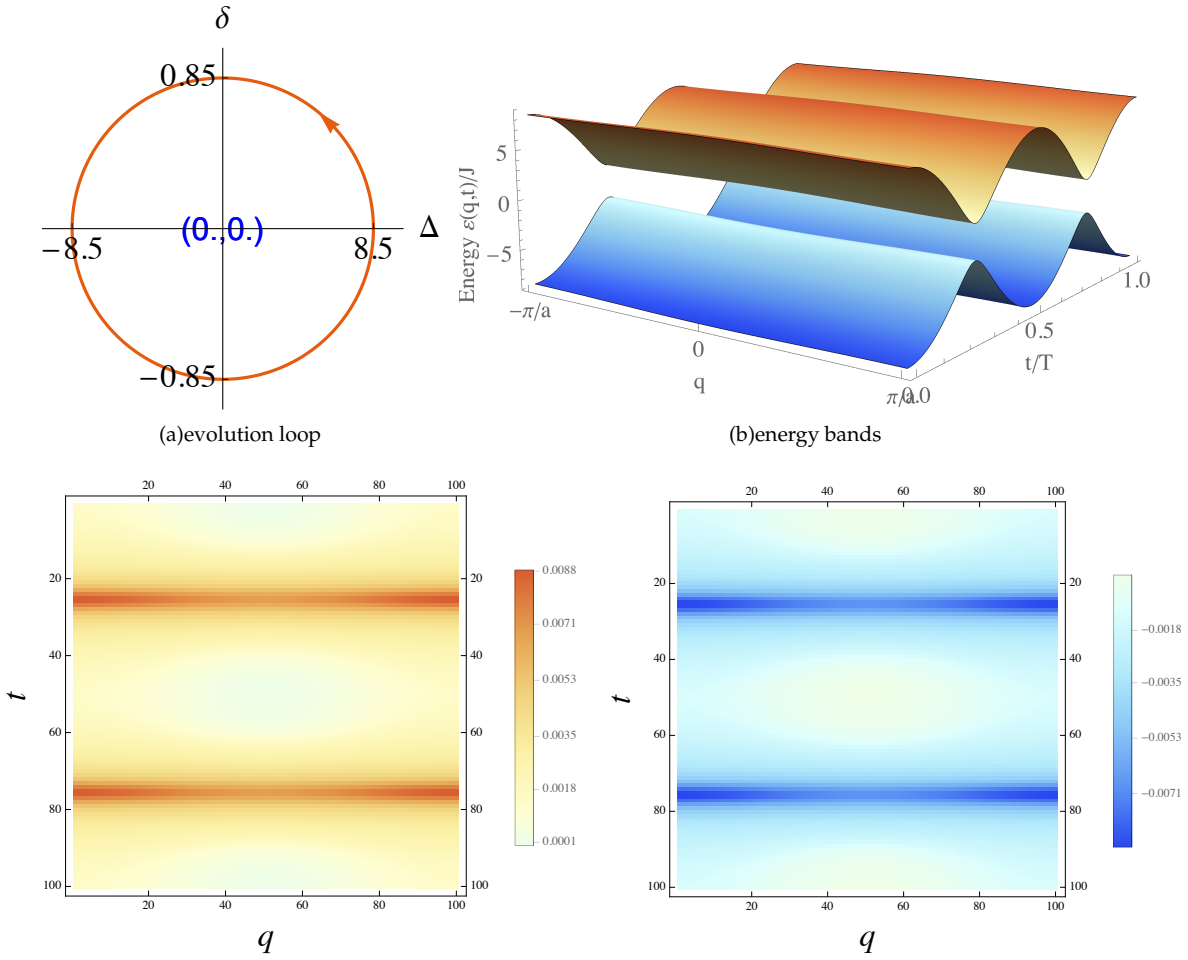
Treating (q,t) as two-dimensional parameter torus, we calculate the Chern number, for each of the two bands, defined by the mapping from this torus to a sphere through the direction of eigenvectors for each band [see Eq. (1)], using the algorithm stated in Sec. I.

a. A typical evolution loop corresponding to parameters in Ref.[4]

$$\begin{aligned}\delta_0 &= 0 & \delta/J &= 0.85 \\ \Delta_0 &= 0 & \Delta/J &= 8.5\end{aligned}$$

Chern number for two bands are calculated as $c_1 = 1$ (lower band), $c_2 = -1$ (upper band).

b. Several other evolution loops listed here



(a)evolution loop (b)energy bands

(c)Berry curvature for lower band (d)Berry curvature for upper band

FIG. 3: Berry field for a typical evolution loop. Degeneracy point $(\delta = 0, \Delta = 0)$ is enclosed by the loop.

Note that the "FrameTicks" N is the number of discretization.

III. COUPLED-SSH MODEL

Consider a coupled SSH model with two chains. There are several ways of coupling the two chains. However we concentrate here on only a particular one which has been explored in experiment[5]. Hamiltonian for a tight-binding model writes

$$\begin{aligned} H &= H^{(1)}_{ssh} + H^{(2)}_{ssh} + H_{cp} \\ &= \sum_{i=1,2}\sum_{j}\Big[-(J+\delta_i)a^\dagger_{ij}b_{ij} - (J-\delta_i)a^\dagger_{ij+1}b_{ij} + h.c.\Big] \\ &\quad + \sum_{j} -t_0\Big[a^\dagger_{1j}a_{2j} + a^\dagger_{1j}b_{2j} + b^\dagger_{1j}b_{2j} + b^\dagger_{1j}a_{2j+1} + h.c.\Big] \end{aligned}$$

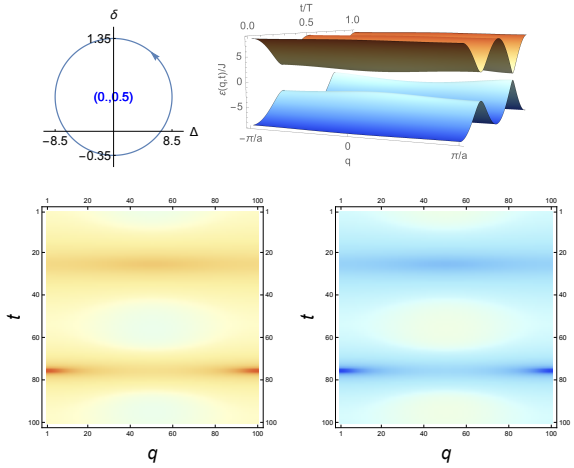


FIG. 4: Degeneracy point is enclosed. $c_1 = 1, c_2 = -1$

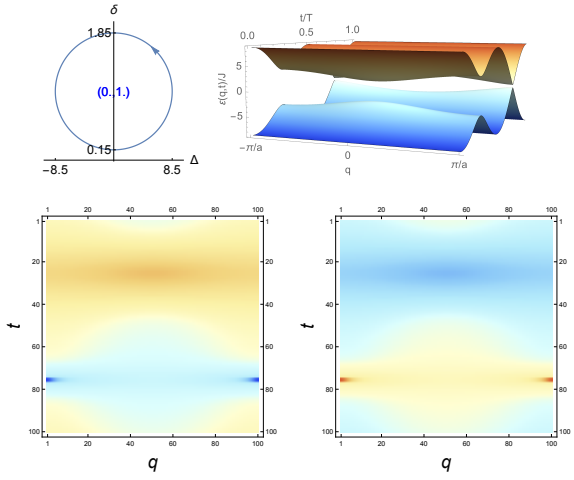


FIG. 5: $(\delta = 0, \Delta = 0)$ is not enclosed. $c_1 = 0, c_2 = 0$

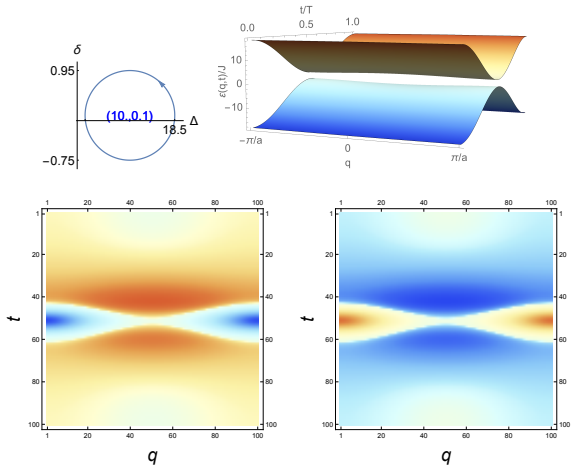


FIG. 6: $(0,0)$ not enclosed. $c_1 = 0, c_2 = 0$

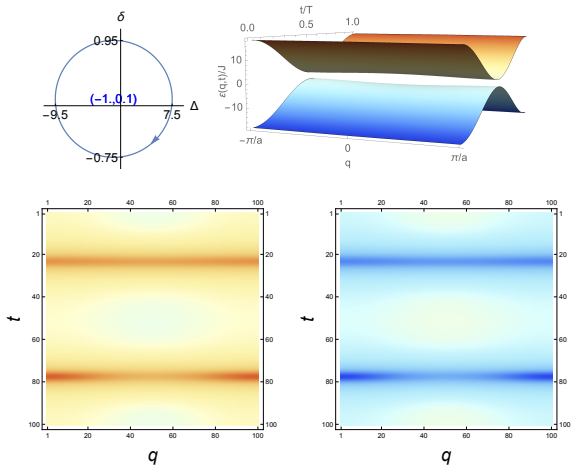


FIG. 7: $(0,0)$ enclosed. Counterclock. $c_1 = -1, c_2 = 1$

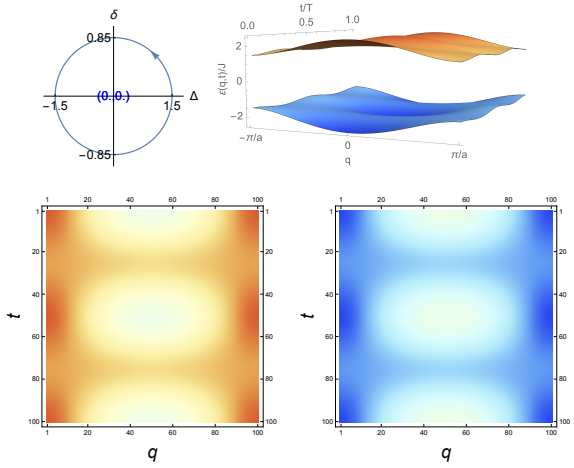


FIG. 8: $(0,0)$ enclosed. With different parameter amplitude $\delta = 0.85, \Delta = 1.5$; $c_1 = 1, c_2 = -1$

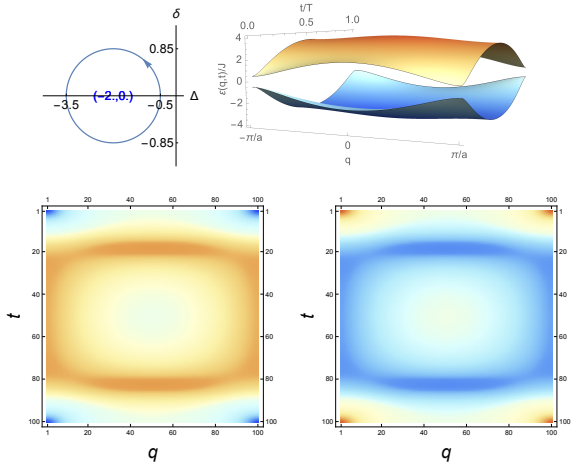


FIG. 9: $(0,0)$ not enclosed. $\delta = 0.85, \Delta = 1.5$. Chern number $c_1 = 0, c_2 = 0$

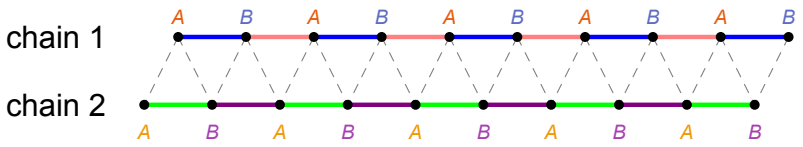


FIG. 10: Schematic diagram of coupled two SSH chains.

Fourier transformed into (crystal) momentum space, the Hamiltonian is of a 4-bands form:

$$\mathcal{H}(q) = \begin{bmatrix} \boldsymbol{h}^{(1)}_{ssh}(q)\cdot\boldsymbol{\sigma} & \boldsymbol{h}_{cp}(q)\cdot\boldsymbol{\sigma} \\ \boldsymbol{h}^{*}_{cp}(q)\cdot\boldsymbol{\sigma} & \boldsymbol{h}^{(2)}_{ssh}(q)\cdot\boldsymbol{\sigma} \end{bmatrix}$$
$$= \begin{bmatrix} 0 & -2J\cos\frac{qa}{2} - \mathrm{i}2\delta_1\sin\frac{qa}{2} & -t_0 e^{-\mathrm{i}qa/4} & -t_0 e^{\mathrm{i}qa/4} \\ -2J\cos\frac{qa}{2} + \mathrm{i}2\delta_1\sin\frac{qa}{2} & 0 & -t_0 e^{\mathrm{i}qa/4} & -t_0 e^{-\mathrm{i}qa/4} \\ -t_0 e^{\mathrm{i}qa/4} & -t_0 e^{-\mathrm{i}qa/4} & 0 & -2J\cos\frac{qa}{2} - \mathrm{i}2\delta_2\sin\frac{qa}{2} \\ -t_0 e^{-\mathrm{i}qa/4} & -t_0 e^{\mathrm{i}qa/4} & -2J\cos\frac{qa}{2} + \mathrm{i}2\delta_2\sin\frac{qa}{2} & 0 \end{bmatrix}$$

a. About the donation:

$$\begin{aligned} \boldsymbol{h}^{(j)}_{ssh}(q) &= (0, -2J\cos\frac{qa}{2}, 2\delta_j\sin\frac{qa}{2}, \Delta_j) \\ \boldsymbol{h}_{cp}(q) &= (-t_0 e^{-\mathrm{i}qa/4}, -t_0 e^{\mathrm{i}qa/4}, 0, 0) \\ \boldsymbol{\sigma} &= (\sigma_0, \sigma_1, \sigma_2, \sigma_3) \\ &= (\mathbb{1}^{(2)}, \sigma_x, \sigma_y, \sigma_z) \end{aligned}$$

Here, for simplicity, as well as consistency with the experiment carried out in Ref.[5], we set $\Delta_j = 0$. That is, no difference in chemical potential for A, B sublattices.

b. Time evolution loop We set up an evolution loop through a periodic time dependency on δ_1 and δ_2. A typical one is

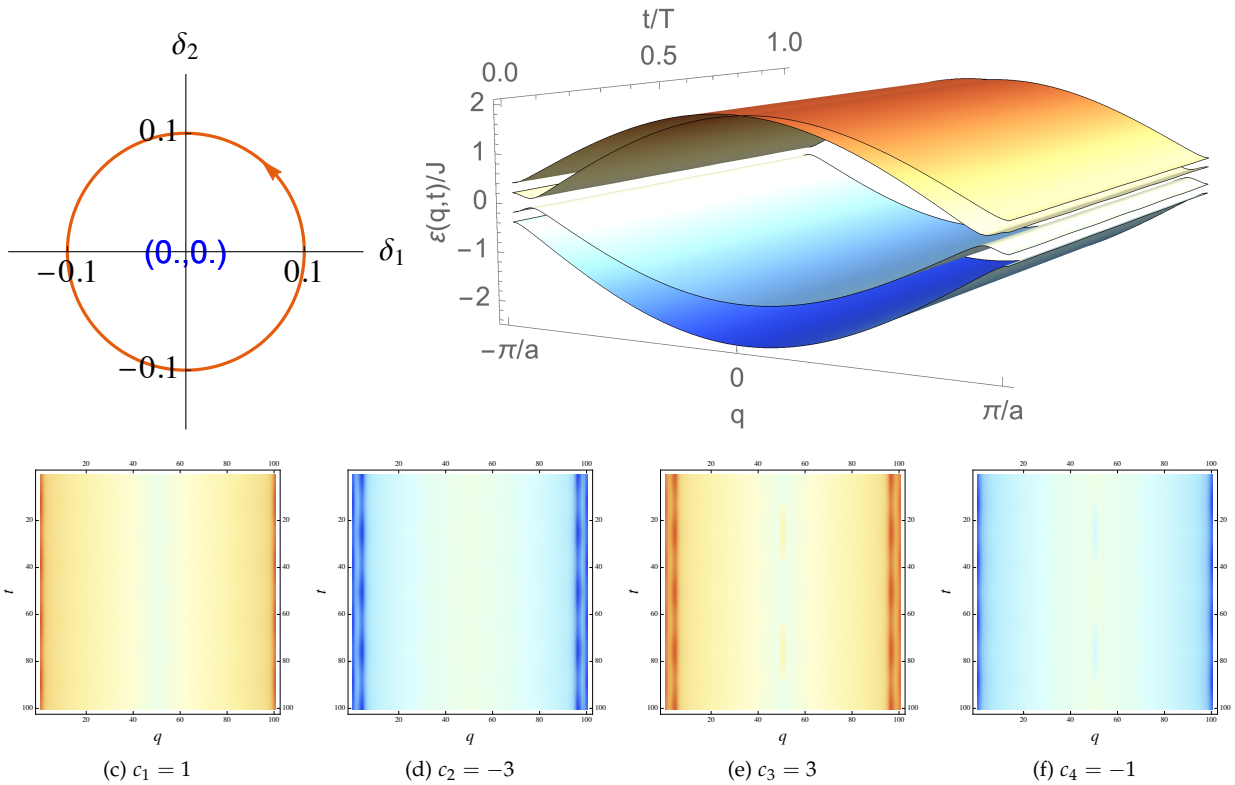
$$\begin{aligned} \delta_1(t) &= \delta_{1o} + \delta_1\cos(\omega t) \\ \delta_2(t) &= \delta_{2o} + \delta_2\sin(\omega t) \end{aligned}$$

Similarly, degeneracy occurs, if allowed, where both $\delta_1, \delta_2 = 0$. The condition for this to happen is $|\delta_{1o}| < |\delta_1|$ and $|\delta_{2o}| < |\delta_2|$.

c. A typical evolution loop closely related to Ref.[5]

Depending on whether or not enclosing the degeneracy point $(\delta_1 = 0, \delta_2 = 0)$, evolution direction (clockwise or counterclockwise), and also band touching or not, we find several different quantum phases distinguished by Chern number for these four bands, which are listed in Table.

d. Several other cases listed here

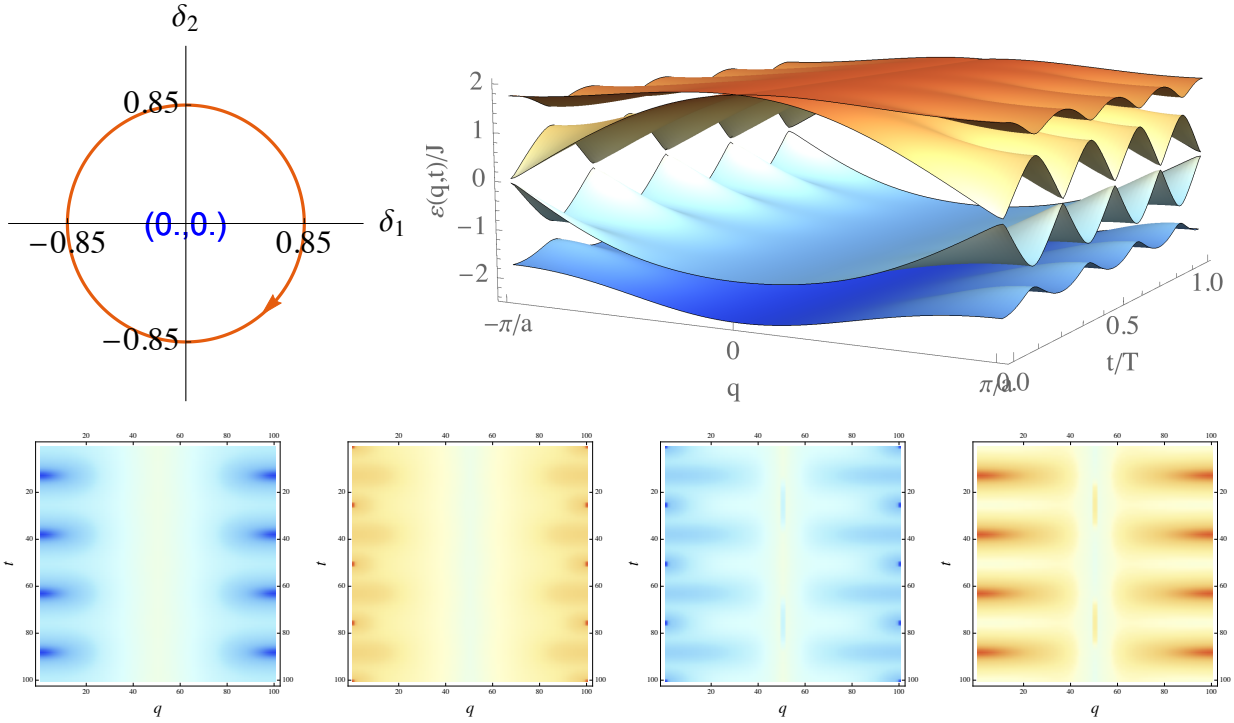


(c) $c_1 = 1$ (d) $c_2 = -3$ (e) $c_3 = 3$ (f) $c_4 = -1$

FIG. 11: Here parameters are $J = 1.0$, $t_0/J = 0.2$, $\delta_1/J = 0.1$, $\delta_2/J = 0.1$

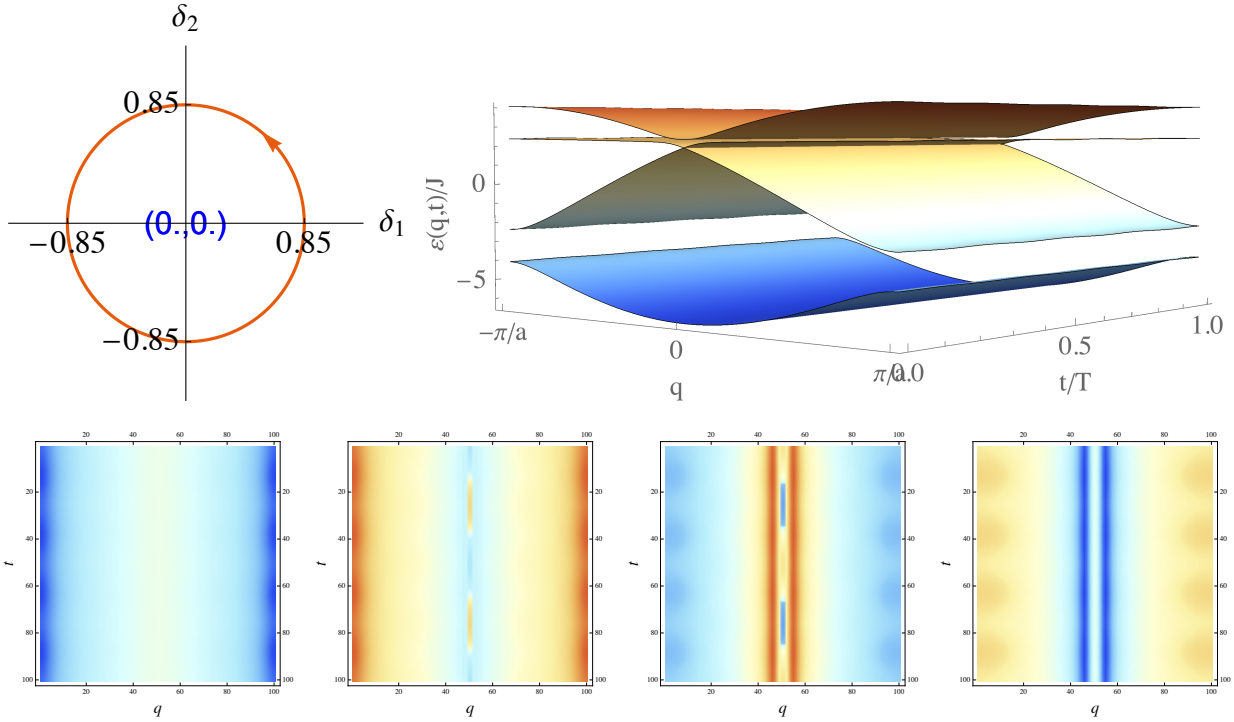
TABLE I: Chern number for coupled-SSH model

Chern number	c_1	c_2	c_3	c_4
Counter-clockwise	1	-3	3	-1
Clockwise	-1	3	-3	1
Not enclosed	0	0	0	0
Middel bands touching	1	-1	-1	0
...				



(c) $c_1 = -1$ (d) $c_2 = 3$ (e) $c_3 = -3$ (f) $c_4 = 1$

FIG. 12: Here parameters are $J = 1.0,\ t_0 = 0.2,\ \delta_1 = 0.85,\ \delta_2 = -0.85$. Clockwise evolution.



(c) $c_1 = -1$ (d) $c_2 = 3$ (e) $c_3 = -3$ (f) $c_4 = 1$

FIG. 13: Here parameters are $J = 1.0,\ t_0 = 2.2,\ \delta_1 = 0.85,\ \delta_2 = 0.85$. Middlemost two bands touch each other.

Elsewhere, if there are band closing during a loop evolution, Chern number could not be calculated (defined) well. Such situations are quite complicated, depending on the setup of parameters.

---

[1] T. Fukui, Y. Hatsugai, and H. Suzuki, *Chern Numbers in Discretized Brillouin Zone: Efficient Method of Computing (Spin) Hall Conductances*, J. Phys. Soc. Jpn. **74** 1674 (2005).

[2] Di Xiao, Ming-Che Chang, and Qian Niu, *Berry phase effects on electronic properties*, Rev. Mod. Phys. **82**, 1959 (2010).

[3] M. J. Rice and E. J. Mele, *Elementary Excitations of a Linearly Conjugated Diatomic Polymer*, Phys. Rev. Lett. **49**, 1455 (1982).

[4] Yoshiro Takahashi's group, *Topological Thouless pumping of ultracold fermions*, Nat. Phys. **12** 296300 (2016).

[5] Sangmo Cheon, Tae-Hwan Kim, Sung-Hoon Lee, Han Woong Yeom, *Chiral solitons in a coupled double Peierls chain*, Science **350**, 6257 (2015).