Lecture notes on topological insulators

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CONTENTS

I. MODERN THEORY OF CHARGE POLARIZATION

In addition to the quantum Hall effect, Berry phase is crucial to the calculation of charge polarization in covalent solids. We explore their connection in this Lect.

A. Charge polarization

The electric polarization $\mathbf{P}$ of a *finite* crystal depends crucially on the charge accumulation near surfaces, and thus cannot be defined as a bulk property. On the other hand, for an *infinite* crystal, the calculation of $\mathbf{P}$, which is the expectation value of $q\mathbf{r}$, diverges.

For a crystal with periodic boundary condition (PBC), $\mathbf{P}$ is generically not well defined. The reason is that, in a periodic solid, the electric polarization depends on one's choice of the unit cell (see Fig. 1). The theory of electric polarization in conventional textbooks applies only to solids consisting of well localized charges, such as ionic or molecular solids (**Clausius-Mossotti theory**).

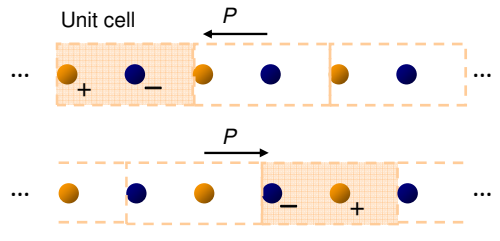

FIG. 1 For an infinite lattice, or a lattice with periodic boundary condition, the polarization is ill-defined. It depends on the choice of the unit cells.

It fails, for example, in a covalent solid with bond charges such that no natural unit cell can be defined.

A crucial observation made by R. Resta is that, even though the value of $\mathbf{P}$ may be ambiguous, its *change* is well defined (Resta, 1992). It was soon pointed out by King-Smith and Vanderbilt that $\Delta\mathbf{P}$ has a deep connection with the Berry phase of the Bloch state (King-Smith and Vanderbilt, 1993).

To illustrate the modern theory of polarization, let's consider a one-dimensional (1D) lattice with periodic boundary condition. There are N lattice points located at $R_\ell = \ell a$ ($\ell \in Z$), and a is the lattice constant. The Fourier transformation of the Bloch state $\psi_{nk} = e^{ikx}u_{nk}$ is called the **Wannier state**,

$$|nR_\ell\rangle = \frac{1}{\sqrt{N}} \sum_{k=-\pi/a}^{\pi/a} e^{-ikR_\ell}|\psi_{nk}\rangle, \tag{1.1}$$

which is localized near a lattice point R_ℓ. The Bloch states form an orthonormal basis,

$$\langle\psi_{n'k'}|\psi_{nk}\rangle = \delta_{nn'}\delta_{kk'}. \tag{1.2}$$

Likewise, the Wannier states are also orthonormal to each other,

$$\langle n'R'|nR\rangle = \delta_{nn'}\delta_{RR'}. \tag{1.3}$$

Like Bloch states, the Wannier states $\{|n\mathbf{R}\rangle, \forall\, \mathbf{R}\}$ form a complete set of bases. A crucial difference is that the former is extended in space, while the latter is localized. With the Wannier states, one can avoid the problem of divergence when calculating the electric polarization.

In an insulator, electric polarization can be related to the *charge center* of the Wannier function,

$$P = q \sum_{\text{filled } n} \langle n0|x|n0\rangle,\ q = -e \tag{1.4}$$

$$= \frac{q}{N}\sum_n \sum_{kk'} \langle u_{nk'}|e^{-ik'x}\frac{1}{i}\frac{\partial}{\partial k}\left(e^{ikx}\right)|u_{nk}\rangle \tag{1.5}$$

$$= \frac{q}{N}\sum_n \sum_{kk'} \langle u_{nk'}|e^{i(k-k')x} i\frac{\partial}{\partial k}|u_{nk}\rangle. \tag{1.6}$$

Decompose the x-integral as a sum of N unit-cell integrals, and write $x = ma + \tilde{x}$ ($\tilde{x} \in [0, a]$), it can be shown

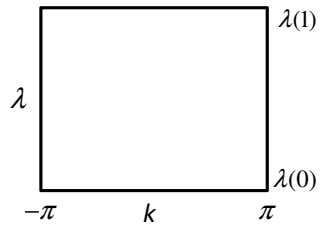

FIG. 2 The domain of Bloch momentum k and parameter λ is similar to a BZ of a two dimensional lattice.

that (see Nomura, 2013, p.85)

$$\langle u_{nk'}|e^{i(k-k')x}i\frac{\partial}{\partial k}|u_{nk}\rangle = N\delta_{k,k'}\langle u_{nk}|i\frac{\partial}{\partial k}|u_{nk}\rangle_{cell} \quad (1.7)$$

$$= \delta_{k,k'}\langle u_{nk}|i\frac{\partial}{\partial k}|u_{nk}\rangle, \quad (1.8)$$

where $\langle\cdots\rangle_{cell}$ integrates over only one unit cell, and $N\langle\cdots\rangle_{cell} = \langle\cdots\rangle$ is used in the second equation. Therefore,

$$P = \frac{q}{N}\sum_n\sum_k\langle u_{nk}|i\frac{\partial}{\partial k}|u_{nk}\rangle \quad (1.9)$$

$$= qa\sum_n\int_{-\pi/a}^{\pi/a}\frac{dk}{2\pi}A_n(k). \quad (1.10)$$

Under a gauge transformation, $|u'_{nk}\rangle = e^{i\chi_{nk}}|u_{nk}\rangle$, where χ_{nk} is single-valued (mod 2π), the polarization contributed from band-n becomes,

$$P'_n = P_n - qa\frac{\chi_{n\pi/a} - \chi_{n-\pi/a}}{2\pi}. \quad (1.11)$$

Single-valuedness of $e^{\chi_{nk}}$ gives $\chi_{nk+2\pi/a} = \chi_{nk} + 2\pi ma$ ($m \in Z$). Therefore,

$$P'_n = P_n - qma. \quad (1.12)$$

The polarization could change by qma under a gauge transformation. That is, only the fractional part of P_n (and P) is gauge invariant.

1. Zak phase

Note that the integral in Eq. (1.10) is nothing but the Berry phase around the BZ divided by 2π,

$$P = qa\sum_n\frac{\gamma_n}{2\pi}. \quad (1.13)$$

The Berry phase of 1D Bloch state is first studied by Zak, 1989 and is called **Zak phase**. In addition to being gauge dependent, the value of Zak phase is also coordinate dependent (see Prob. 1), but the relative phases between energy bands are fixed.

For a 1D lattice with *space inversion* symmetry, if the origin is at a symmetric point, then the Zak phase can only be 0 or π, and P_n can only be 0 or $qa/2$. This can be understood as follows: It was shown earlier that if the lattice has space inversion symmetry, then (see Eq. (**??**))

$$A_n(-k) = -A_n(k). \quad (1.14)$$

Therefore, after the inversion,

$$P_n \to P'_n = qa\int_{-\pi/a}^{\pi/a}\frac{dk}{2\pi}A_n(-k) = -P_n. \quad (1.15)$$

Since P_n is allowed to have the freedom of changing by qma, the constraint given by the inversion symmetry is

$$P_n = -P_n \mod qa \quad (1.16)$$

$$\to P_n = 0 \text{ or } q\frac{a}{2} \mod qa. \quad (1.17)$$

Put it in another way, for a lattice with space-inversion symmetry, the charge center $\langle n0|x|n0\rangle$ in a unit cell can only be at 0 or $a/2$. That is, on top of a lattice point or in the middle between two lattice points.

On the other hand, if there is no inversion symmetry, then γ_n (and P_n) can be any value. An experimental confirmation of the Zak phase with cold atoms can be found in Atala *et al.*, 2013.

2. Quantized charge pump

Even though P_n is gauge dependent, the change of polarization ΔP_n under an adiabatic and continuous deformation is gauge invariant and well-defined. From here on we consider only one filled band, and use λ to label the degree of ion displacement (with respect to ions of opposite charge). It varies from 0 to a as the ions shift adiabatically from an initial position to a final position.

The difference of polarizations between these two states is,

$$P(\lambda_2) - P(\lambda_1) = qa\int_{-\pi/a}^{\pi/a}\frac{dk}{2\pi}\left[A(k,\lambda_2) - A(k,\lambda_1)\right]. \quad (1.18)$$

The parameter λ defines a second dimension in addition to k. We can choose the parallel transport gauge (see Chap **??**), such that along the λ-direction,

$$\langle u_{nk}|\frac{\partial}{\partial\lambda}|u_{nk}\rangle = 0, \quad (1.19)$$

then ΔP can be written as a (counter-clockwise) line integral around the rectangle in Fig. 2,

$$\Delta P = -\frac{qa}{2\pi}\oint d\mathbf{k}\cdot\mathbf{A}(\mathbf{k}), \quad \mathbf{k}\equiv(k,\lambda) \quad (1.20)$$

$$= -\frac{qa}{2\pi}\int d^2k F_z(\mathbf{k}), \quad (1.21)$$

where $F_z(\mathbf{k}) = \partial_k A_\lambda - \partial_\lambda A_k$, and $A_\lambda = i\langle u_{\mathbf{k}}|\partial_\lambda|u_{\mathbf{k}}\rangle$.

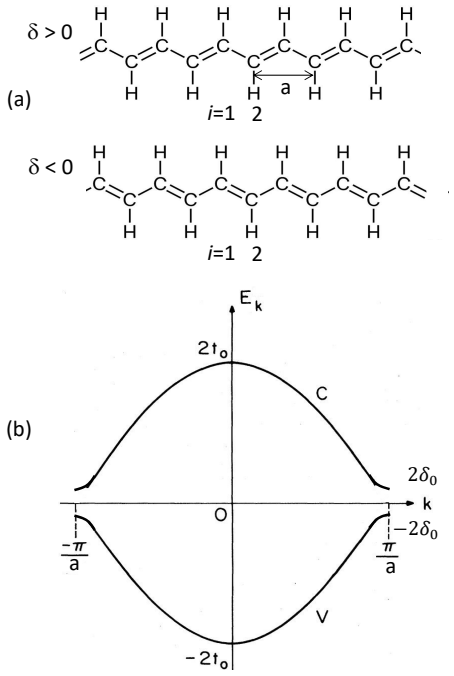

FIG. 3 (a) Two different locations of double bonds in trans-polyacetylene. (b) Conduction band and valence band of the SSH model.

If $\lambda(1) = \lambda(0)$, then the rectangle is similar to a BZ, where opposite edges habor the same states. Therefore, the integral of the Berry curvature is an integer ($\times 2\pi$), and

$$\Delta P = qaC_1. \tag{1.22}$$

That is, under a cyclic parametric variation, the charge transport is "quantized". This fact can be utilized to build a **quantized charge pump** (Thouless *et al.*, 1982). However, be aware that even though the quantization is precise in the adiabatic limit, it is no longer so if the pumping is fast.

The analysis above is based on one-particle states in 1D. But the same scheme can be extended to real solids with electronic interactions in three dimensions. An essential alteration is to replace the one-particle states by the **Kohn-Sham orbitals** in the **density functional theory** (King-Smith and Vanderbilt, 1993).

B. Su-Schrieffer-Heeger model

To explore the Zak phase in 1D systems, we study the Su- Schrieffer-Heeger (SSH) model of polyacetylene. It starts with the tight-binding model (Su *et al.*, 1979),

$$H_{SSH} = \sum_{i=1}^{2N} \left(t_0 + (-1)^i \delta\right) \left(c_i^\dagger c_{i+1} + h.c.\right), \tag{1.23}$$

where t_0 is the hopping amplitude between nearest neighbors, and $\pm\delta$ modulate the hopping strength (see Fig. 3(a)). We impose the **periodic boundary condition** (PBC), so that $c_{2N+1} = c_1$, and electron spins are ignored for now.

Since the lattice is dimerized, it is convenient to write $c_{i=2j-1}$ as c_j, $c_{i=2j}$ as d_j, and double the size of the unit cell. The Hamiltonian becomes,

$$H_{SSH} = \sum_{j=1}^{N} t_- \left(d_j^\dagger c_j + h.c.\right) + \sum_{j=1}^{N} t_+ \left(c_{j+1}^\dagger d_j + h.c.\right), \tag{1.24}$$

where $t_\pm \equiv t_0 \pm \delta$. Expand c_j and d_j,

$$c_j = \frac{1}{\sqrt{N}} \sum_k e^{ijak} c_k, \tag{1.25}$$

$$d_j = \frac{1}{\sqrt{N}} \sum_k e^{ijak} d_k, \tag{1.26}$$

where N is the total number of unit cells, and a is the lattice constant, then

$$\begin{aligned} H_{SSH} &= \sum_k (c_k^\dagger, d_k^\dagger) \begin{pmatrix} 0 & t_- + t_+ e^{-iak} \\ t_- + t_+ e^{+iak} & 0 \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix} \\ &= \sum_k (c_k^\dagger, d_k^\dagger) \mathsf{H}(k) \begin{pmatrix} c_k \\ d_k \end{pmatrix}. \end{aligned} \tag{1.27}$$

Write $\mathsf{H}(k) = \mathbf{h}(k) \cdot \boldsymbol{\sigma}$, then

$$\mathbf{h}(k) = (t_- + t_+ \cos ka, t_+ \sin ka, 0). \tag{1.28}$$

The eigenenergies are

$$\varepsilon_\pm(k) = \pm|\mathbf{h}(k)| = \pm 2 \left(t_0^2 \cos^2 \frac{ka}{2} + \delta^2 \sin^2 \frac{ka}{2}\right)^{1/2}. \tag{1.29}$$

The two energy bands are separated by an energy gap $4|\delta|$ (Fig. 3(b)). The energy gap closes when $(ka, \delta) = (\pm\pi, 0)$.

1. Zak phase

Note that the Hamiltonian H has the same structure as the one for the spin-1/2 system in Eq. (**??**), with $\mathbf{h}(k)$ playing the role of the magnetic field. The two sublattices correspond to the spin up/down degrees of freedom. Therefore, the Berry phase (or Zak phase here) due to the evolution of k around the 1D Brillouin zone equals *half* of the solid angle extended by a closed path in the **h**-space. Since $h_z(k) = 0$, the path is lying on the $h_x - h_y$ plane.

If $\delta > 0$ (i.e. $t_+ > t_-$), then when k runs across the BZ, the trajectory of $\mathbf{h}$ encircles the origin (path-1 in Fig. 5(a)). The solid angle of path-1 with respect to the origin is 2π, and the Zak phase is π, half of the solid angle. On the other hand, if $\delta < 0$ ($t_+ < t_-$), then $\mathbf{h}$ follows path-3 that does not encircle the origin. The

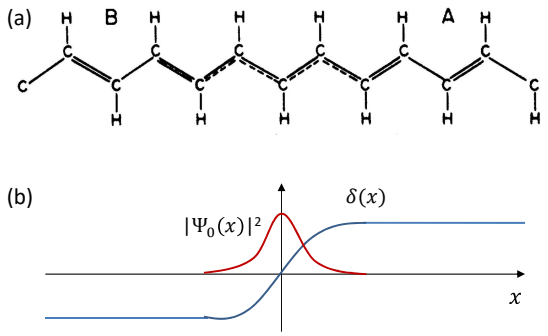

FIG. 4 (a) The junction between two phases in the SSH model. (b) The localized state trapped in the domain wall. The characteristic length of $\delta(x)$ is much larger than the lattice constant.

solid angle of path-3 with respect to the origin is zero, and the Zak phase is zero.

That is, there are two different phases in the SSH model. To change from one phase to the other, δ needs to cross the value of zero, when the energy gap closes.

2. Domain wall state

Assume a SSH chain has two domains: $\delta(x) = -\delta_0 < 0$ for $x \ll 0$, $\delta(x) = \delta_0$ for $x \gg 0$ (Fig. 4(a)), and $\delta(x)$ varies smoothly and monotonically from $-\delta_0$ to δ_0 in between. We will show that there is a localized state trapped in this domain wall.

The low-energy states are located near $ka = \pm\pi$. Write k as $\pi/a + q$, and expand $\mathsf{H}(k)$ to linear order in q, then the Hamiltonian matrix becomes

$$\begin{aligned} \mathsf{H} &\simeq 2\begin{pmatrix} 0 & -\delta + it_+ q\frac{a}{2} \\ -\delta - it_+ q\frac{a}{2} & 0 \end{pmatrix} \\ &= -2\delta(x)\ \sigma_x - t_+(x) qa\ \sigma_y. \end{aligned} \tag{1.30}$$

This is the Hamiltonian in the continuum limit: the wavelength of an electron is much larger then the lattice constant (but smaller than the characteristic length of the profile of $\delta(x)$). To study the electronic states in this non-uniform chain, we can replace q by $(1/i)\partial/\partial x$ to *requantize* the system. Such a semiclassical approach is used widely, for example, in finding the bound states of an impurity atom in semiconductor.

After requantization, the Schrödinger equation is

$$\begin{pmatrix} 0 & -2\delta + t_+ a\frac{d}{dx} \\ -2\delta - t_+ a\frac{d}{dx} & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}. \tag{1.31}$$

We are interested in the mid-gap state with $E = 0$. It is not difficult to confirm that the eigenstate with zero energy is

$$\Psi_0(x) = e^{-\int_0^x dx' \frac{2}{t_+(x')a}\delta(x')} \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \tag{1.32}$$

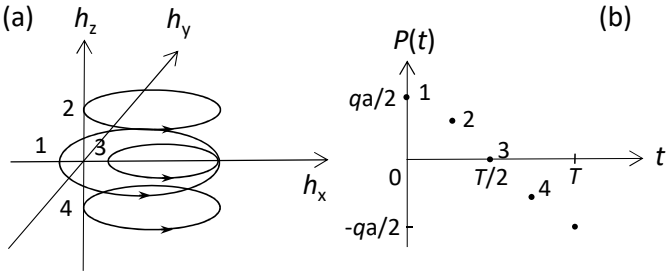

FIG. 5 (a) The trajectory of $\mathbf{h}(k)$ evolves in the order of 1, 2, 3, 4, when $t = 0, T/4, T/2, 3T/4$. (b) The evolution of electric polarization for the 4 steps in (a).

This is a state localized in the domain wall around $x = 0$ (see Fig. 4(b)). It would not disappear without destroying the domain wall all together.

A recent experimental work about the trapped state can be found in Meier *et al.*, 2016. Note: Jackiw and Rebbi, 1976 are the first to study this problem, albeit in the context of high-energy physics.

C. Rice-Mele model

To illustrate the parametric charge pumping, we consider the **Rice-Mele model**, which is an extension of the SSH model (Rice and Mele, 1982),

$$H = H_{SSH} + \sum_{j=1}^{N} \Delta c_j^\dagger c_j - \sum_{j=1}^{N} \Delta d_j^\dagger d_j, \tag{1.33}$$

where $\pm\Delta$ are the on-site potentials for staggered sublattices. Following the same procedure in the study of the SSH model, write the Hamiltonian in momentum basis,

$$H = \sum_k (c_k^\dagger, d_k^\dagger) \begin{pmatrix} \Delta & t_- + t_+ e^{-iak} \\ t_- + t_+ e^{+iak} & -\Delta \end{pmatrix} \begin{pmatrix} c_k \\ d_k \end{pmatrix}. \tag{1.34}$$

This gives

$$\mathbf{h}(k) = (t_- + t_+ \cos ka, t_+ \sin ka, \Delta), \tag{1.35}$$

and the band energies are

$$\varepsilon_\pm(k) = \pm\left(\Delta^2 + 4t_0^2 \cos^2\frac{ka}{2} + 4\delta^2 \sin^2\frac{ka}{2}\right)^{1/2}. \tag{1.36}$$

We now consider a cyclic variation,

$$(\delta(t), \Delta(t)) = \left(\delta_0 \cos 2\pi\frac{t}{T}, \Delta_0 \sin 2\pi\frac{t}{T}\right). \tag{1.37}$$

When t evolves through a period T, $\mathbf{h}(k)$ ($k \in [0, 2\pi/a]$) traverses paths 1, 2, 3, 4 and back to 1 in Fig. 5(a). For each loop, the Berry phase equals *half* of the solid angle extended by the loop in the $\mathbf{h}$-space. The polarization

$P = qa\gamma/2\pi$ is shown in Fig. 5(b). After a full cycle, P changes by qa (mod qa). That is, a quantized charge q could be transported with a distance a. This works as a quantized charge pump. Experimental confirmations of the charge pumping related to the Rice-Mele model can be found in Lohse *et al.*, 2015, and Nakajima *et al.*, 2016.

Exercise

1. The value of Zak phase depends on the choice of the origin. Under a shift of the origin,

$$\psi_k(x) \to \psi'_k(x) = \psi_k(x-d). \tag{1.38}$$

This leads to

$$u_k(x) \to u'_k(x) = u_k(x-d)e^{-ikd}. \tag{1.39}$$

Show that

$$\gamma \to \gamma' = \gamma + 2\pi\frac{d}{a}, \tag{1.40}$$

where a is the lattice constant.

2. The $\mathbf{h}(k)$ of SSH model traces out a loop in the $\mathbf{h}$-space when k runs through the first Brillouin zone.
(a) Show that the following expression gives the winding number of the loop around the origin,

$$w = \frac{1}{2\pi}\int_{BZ} dk\ \frac{1}{h^2}\hat{\mathbf{z}}\cdot\mathbf{h}\times\frac{d\mathbf{h}}{dk}. \tag{1.41}$$

(b) The SSH Hamiltonian can be written as,

$$\mathsf{H}(k) = \begin{pmatrix} 0 & Q(k) \\ Q^*(k) & 0 \end{pmatrix}, \tag{1.42}$$

where $Q(k) = h_x - ih_y$. Show that the following expression also gives the winding number of $\mathbf{h}(k)$ around the origin,

$$w = \frac{i}{2\pi}\int_{BZ} dk\frac{d}{dk}\ln Q(k). \tag{1.43}$$

3. The reflection operator for the SSH model can be written as $\Pi = \sigma_x$.
(a) Show that the SSH model has the reflection symmetry,

$$\Pi^\dagger\mathsf{H}(k)\Pi = \mathsf{H}(-k). \tag{1.44}$$

What are the restrictions of this relation on the three components of $\mathbf{h}(k)$?
(b) Show that when there is reflection symmetry, the electric polarization needs to be quantized, $P = 0$ or $qa/2$.

4. It is known that when $ka = 0, \pi$,

$$\mathsf{H}(0) = 2t_0\ \sigma_x, \mathsf{H}(\pi) = -2\delta\ \sigma_x. \tag{1.45}$$

At these two points, H commutes with the reflection operator Π, hence the parity ξ of Π can be well-defined.
(a) Show that for the valence band,

$$\xi(0) = -1, \xi(\pi) = \mathrm{sgn}(\delta), \tag{1.46}$$

in which $\mathrm{sgn}(\delta)$ is the sign of δ.
(b) Let ν be the product of two parities,

$$\nu = \xi(0)\xi(\pi). \tag{1.47}$$

What are the values of ν when $\delta > 0$ and $\delta < 0$? This shows that the topology described by the winding number of $\mathbf{h}$ or the Zak phase can also be characterized by the product of the parities of filled states at $ka = 0, \pi$.

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