Static electric field in one-dimensional insulators without boundaries

Kuang-Ting Chen and Patrick A. Lee

Phys. Rev. B **84**, 113111 — Published 26 September 2011

DOI: 10.1103/PhysRevB.84.113111

Static Electric Field in 1D Insulators without Boundaries

Kuang-Ting Chen[1] and Patrick A. Lee[1]

[1] *Department of Physics, Massachusetts Institute of Technology, Cambridge, MA 02139*

(Dated: September 2, 2011)

In this brief report, we show that in a 1D insulating system with periodic boundary conditions, the coefficient of the θ-term in the effective theory is not only determined by the topological index, $\int i \sum_{\alpha\in\text{occ}} \langle u_{k\alpha}| \frac{\partial}{\partial k} |u_{k\alpha}\rangle \, \mathrm{d}k$. Specifically, the relative position between the electronic orbitals and the ions also alters the coefficient, as one would expect when one identifies $(-e\theta/2\pi)$ as the polarization. This resolves a paradox when we apply our previous result to the Su-Shreiffer-Heeger model where the two ground states related by a lattice translation have θ differed by π. We also show that the static dielectric screening is the same with or without boundaries, contrary to what we have commented in our previous paper.

I. INTRODUCTION

In our previous paper[1], we argue that in a setting without boundaries, the topological insulator in one dimension (1D) and three dimensions (3D) can still be characterized by a θ-term in the effective theory, which in turn gives measurable consequences. Specifically, in 1D there is a term $(e\theta/2\pi)E$ in the effective Lagrangian, where $(-e\theta/2\pi)$ is usually identified as the polarization P, by comparing the term to the energy density $(-P\cdot E)$. For non-interacting systems, θ is given by

$$\theta = \int i \sum_{\alpha\in\text{occ}} \langle u_{k\alpha}| \frac{\partial}{\partial k} |u_{k\alpha}\rangle \, \mathrm{d}k. \tag{1}$$

We have shown that this term results in a constant electric field $\frac{\theta e}{2\pi}$ in the bulk, provided that the electric field is confined in one dimension.

This observation, however, seems puzzling when one considers the well-known Su-Schreiffer-Heeger (SSH) model[2]. If we consider spinless electrons, the two ground states in this model will have the effective θ-term with θ which differs by π. A naive application of Eq. (1) suggests that the two ground states have different electric fields. On the other hand, the two states are related by a lattice translation of a (where the doubled unit cell is of period $2a$) and are physically identical. They thus cannot have different electric fields. In this report we will resolve this issue.

Another related conceptual problem is whether the static electric field can be screened in a setting without boundaries. Intuitively, one might imagine that the dielectric screening comes from the accumulated charges at the two ends. Without boundaries these charges are absent, and there seems to be no way to screen the electric field. We will, however, show in the following that the electric field in the bulk is screened by the dielectric constant, in the same way as if there are boundary charges. There are two ways to understand the effect. we can either take the screening effect into account from the start, by including the dielectric constant in our formalism. This way we then can derive that it is ϵE which is quantized in integer multiples of e with a shift of $-\theta e/2\pi$. We can also consider instead the feedback of the generated electric field to the θ-term separately, which is more intuitively like a "screening" effect. In this case we find the shift in quantization of E is still given by θ, but the effective θ is shifted back a little bit by the finite electric field it generates. The two description in the end gives the same ground state electric field.

In Sec. II we look into the SSH model, verify the topological index of the ground states. We then explain how we can resolve the apparent contradiction. In Sec. III we explain the dielectric screening effect in the 1D setting without boundaries.

II. THE SSH MODEL, TOPOLOGICAL INDEX, AND THE STATIC ELECTRIC FIELD

The SSH model is given by the following Hamiltonian in 1D[2]:

$$H = \sum_{i,\sigma} (-t + (-1)^i \Delta) c^\dagger_{i\sigma} c_{i+1\sigma} + h.c., \tag{2}$$

Δ takes either positive or negative values for the two ground states which spontaneously break the lattice translation symmetry. Suppose we plug in the wave function

$$\psi_k = a_k \sum_{i\in\text{odd}} c^\dagger_i |0\rangle \exp(ikx_i) + b_k \sum_{j\in\text{even}} c^\dagger_j |0\rangle \exp(ikx_j), \tag{3}$$

The Hamiltonian can be put into a matrix form:

$$H_k \begin{pmatrix} a_k \\ b_k \end{pmatrix} = (-2t\cos(ka)\sigma_x + 2\Delta \sin(ka)\sigma_y) \begin{pmatrix} a_k \\ b_k \end{pmatrix}; \tag{4}$$

σ_x and σ_y are Pauli matrices and a is the lattice spacing. Notice that H_k is *not* periodic in π/a; nevertheless ψ_k is periodic (up to a phase.) When we apply a small electric field, the coupling enters via Peierls substitution, and directly results in $H_k \to H_{k+eA}$, where A is the spatial part of the gauge field. At half filling where the system is insulating, following our previous discussion, we can calculate the Berry's phase accumulated when we adiabatically turn on the electric field until the system reaches the

state related to the initial state by a large gauge transform of winding number one, $A \to A+2\pi/eL$:[3] (hereafter when we write "the Berry's phase" we refer to the Berry's phase of this procedure)

$$\theta_{\text{Berry}} = \int_{-\pi/2a}^{\pi/2a} i \langle u_k | \frac{\partial}{\partial k} | u_k \rangle \, \mathrm{d}k, \tag{5}$$

with $|u_k\rangle = \begin{pmatrix} a_k \\ b_k \end{pmatrix}$, and we choose the phase convention such that ψ_k periodic in k. If we take $x_n = na$, we can parametrize our solution as

$$|u_k\rangle = \exp\left(\frac{i\text{sgn}(\Delta) f(k)}{2}(\sigma_z - 1)\right)\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \tag{6}$$

with

$$\tan(f(k)) = \left|\frac{\Delta}{t}\right| \tan(ka). \tag{7}$$

The important thing here is to notice that $f(k) = 0$ at $k = 0$ and $f(k) = \pm\pi/2$ at $k = \pm\pi/2a$. We therefore get

$$\theta_{\text{Berry}} = \text{sgn}(\Delta)\frac{\pi}{2}, \tag{8}$$

for each spin.

If we consider the spinful case as in the original SSH model, the total Berry's phase is $2\theta_{\text{Berry}}$, which differs 2π from each other for the two ground states, implying that both would have the same properties. However, since $\theta = \pi$ for both states, we would naively predict that there is a electric field $E \sim \pm e/2$ in both states. This prediction seems rather unlikely. For the spinless case, the situation is even worse, as the θ differs by π between the two states, generating a different static electric field. Yet, the two states are related by a lattice translation of a, and should be physically equivalent.

These paradoxical observations can be resolved, if we realize that the charged ions can also have a Berry's phase. It is somewhat surprising in the sense that the ions are considered to be stationary localized charges and behave rather trivially. To see how the Berry's phase comes about, we have to recall how the Berry's phase is properly defined. In order to define the Berry's phase when the state adiabatically transforms into another state which is related to the original state by a large gauge transform, we first have to identify the two states as two different descriptions of the same physical state.[1] Therefore they have to correspond to the same physical state up to a definite phase. Consider a Bloch wave function $\psi_k(x) = u_k(x)\exp(ikx)$, under the large gauge transform of winding number one, it becomes

$$\begin{aligned}\psi_k(x) \to \bar{\psi}_k(x) &= \psi(x)\exp(-i2\pi x/L) \\ &= u_k(x)\exp(i(k-2\pi/L)x);\end{aligned} \tag{9}$$

L is the size of the lattice. Without loss of generality, let us identify the two wave functions (that is, to assume the two wave function describe the same physical state with identical phases):

$$u_k(x)\exp(ikx) \sim u_k(x)\exp(i(k-2\pi/L)x). \tag{10}$$

For consistency, this identification should stay the same for any $u_k(x)$.

Now let us shift both wave functions by x_0:

$$\begin{aligned}\psi'_k(x) &= u_k(x-x_0)\exp(ik(x-x_0)) \\ &= (u_k(x-x_0)\exp(-ikx_0))\exp(ikx) \\ &\equiv u'_k(x)\exp(ikx).\end{aligned} \tag{11}$$

$$\begin{aligned}\bar{\psi}'_k(x) &= u_k(x-x_0)\exp(i(k-2\pi/L)(x-x_0)) \\ &= u'_k(x)\exp(i(k-2\pi/L)x)\exp(i2\pi x_0/L)\end{aligned} \tag{12}$$

We can regard $u'_k(x)$ as the periodic part of some other wave function. Therefore, with the identification Eq. (10), we must have

$$\psi'_k(x) \sim u'_k(x)\exp(i(k-2\pi/L)x) = \bar{\psi}'_k(x)e^{-i2\pi x_0/L}; \tag{13}$$

that is, following the same identification, the translated wave function is identified with the translated gauge transform with an additional phase $\phi = (-2\pi x_0/L)$!

This phase shows up in the calculation of the Berry's phase. We have

$$\begin{aligned}\theta'_{\text{Berry}} &= \int_{-\pi/a}^{\pi/a} i \langle u'_k | \frac{\partial}{\partial k} | u'_k \rangle \, \mathrm{d}k \\ &= \theta_{\text{Berry}} + 2\pi\left(\frac{x_0}{a}\right).\end{aligned} \tag{14}$$

The extra Berry's phase is compensated by the extra phase in Eq. (13), after summing over (L/a) states in the Brillouin zone.

This "non-invariance" of the identification under translation" arises from the fact that the gauge transform does not commute with translation. The discussion above shows that this Berry's phase for a single charged wave function is not a physical quantity. It depends on how one identifies the wave functions related by a large gauge transform; however, for a given identification, the wave functions are identified differently when they are translated.

Nevertheless, the total phase difference in the identification for a product of single particle wave functions when the state are translated by x_0 equals $N\phi$, where N is the total charge. For a charge-neutral system, the total Berry's phase is therefore invariant under the translation of the whole system. Since the translation changes the position of the ions, the Berry's phase, or the coefficient of the θ-term, is not determined only by the "topology" of the occupied bands, but also reflects their relative position to the ionic lattice. A translation of only the electrons or only the ions will result in a different Berry's phase, and a different ground state electric field.

Let us now return back to the original problem. In the spinless case, the ions should have the same density as the electrons, which is half a charge per unit cell. If the

ions are localized, they would have a $2a$ period. For the two degenerate ground state, the ionic states are related by a shifted of a. Now that we know that a half-period shift of the ions will also give a Berry's phase differed by π, the total Berry's phase is indeed the same for the two ground states.

One might wonder how this argument applies for a jellium-like ionic state. The translated ions can look very similar to the original state, and it seems paradoxical for them to have such different Berry's phases. Here we argue that, despite the similarity in the density profile, since we only have one ion per two lattice spacing, the translated state is always very different from the original state, as long as the ions are localized. This is most evident when we look from the single-particle perspective. The center-of-mass positions of the ions must differ by $2a$, and the product wave function is different if we shift it by a. On the other hand, if one thinks about the opposite (unphysical) limit, where the ions are completely delocalized and are described by plane waves, to get rid of any $2a$ periodicity, the ionic state then becomes gapless, and the Berry's phase procedure does not apply. We thus conclude that for an inert ionic lattice with one ion per two lattice spacing, it can only be $2a$-periodic, and a translation of a gives a different state, with a Berry's phase differed by π.

When we derive Eq.(8), it is as if we implicitly assume the ions are setting right at $x_n = 2na$ (so that they do not contribute to the Berry's phase.) If we place the ions at the places where most electrons are, $x_n = \mathrm{sgn}(\Delta)\frac{1}{2}a + 2na$, the total Berry's phase for both ground states are zero. Fig. (1) summarizes the result.

For the spinful case, since the number of ions are doubled, the difference between the Berry's phases of the two states is also doubled. The lattice contribution for the two states therefore differs by 2π, which implies that shifting the lattice by a does not change the ground state property, as expected. To get the correct expression for θ however, we still have to consider the ionic contribution to the Berry's phase. The π Berry's phase we obtained eariler does not include the ionic contribution, which is equivalent to assuming they are placed at $x_n = 2na$, with two ions at the same site. If we shift half of the ions by a, forming the usual lattice with period a, the total Berry's phase will again be shifted by π, and there will be no ground state electric field.

Closing this section, we note that if we view θ as the polarization[3,4], it seems almost trivial to say that it must depend on the ionic lattice. Nevertheless, prior to this work it is unclear how one recovers this dependence on the ionic lattice with periodic boundary conditions, along with Eq. (1). Our argument thus provides a simple picture which complements the conventional view of polarization with open boundaries conditions. It is especially helpful with unit cell doubling, as in the conventional view, the termination of the crystal with doubled unit cell complicates the problem.

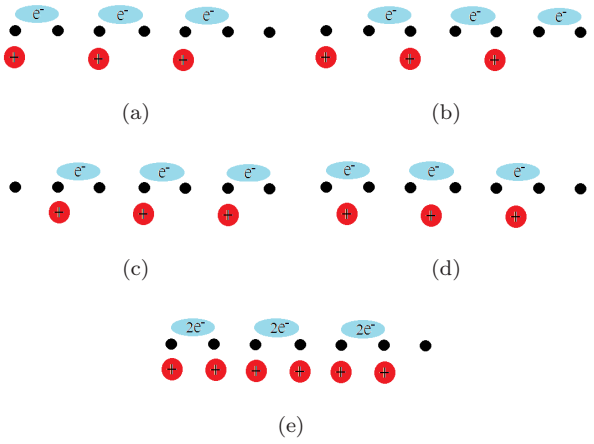

FIG. 1. (a)-(d) refers to the spinless case. (a) One of the electronic "ground state", without considering the ions. It is predicted in this state there is a -e/4 static electric field. (b) The other "ground state", without changing the lattice. Evidently the two state are different. (c) The other ground state with ions shifted. Now the physics is identical to (a). Even though we draw point-like ions here, the argument actually works for any charge distribution, including jellium as a limiting case. (d) If the ions are at the lowest energy positions, the ground state electric field is zero. (e) For the spinful case, a simple consideration would show that this configuration will have zero ground state electric field.

III. THE DIELECTRIC SCREENING

In a one dimensional world, a electric field with magnitude $e/2$ is huge. In a topological insulator with $\theta = \pi$, it is thus natural to ask whether the generated electric field can somehow be screened to lower the total energy, with periodic boundary conditions. In addition, if the electric field is not screened, it then becomes an universal signature of the 1D topological insulator. With open boundary conditions, the static electric field is screened by the dielectric constant. This screening corresponds to a net displacement between the electrons and the ions. With periodic boundary conditions, no charges are accumulated from such displacement; however, from the discussion in the previous section, we now know this displacement changes the θ. We therefore are set to answer the question, whether the screening with periodic boundary conditions is the same as with open boundary conditions.

We first start from an effective theory with a built-in dielectric constant:

$$\mathcal{L}_{1D} = -\frac{\epsilon}{4}(F_{\mu\nu})^2 + \frac{e\theta}{2\pi}\epsilon^{\mu\nu}\partial_\mu A_\nu = \frac{\epsilon}{2}E^2 + \frac{e\theta}{2\pi}E. \quad (15)$$

Let us again write down the $q = 0$ sector of the partition function following our previous paper[1]:

$$Z_{q=0} \propto \int_0^{2\pi} \mathrm{d}\phi \int_{-\infty}^{\infty} \frac{\mathrm{d}\ell}{2\pi} \sum_{\mathrm{m,n}} \langle \phi + 2\pi \mathrm{m}|\ell\rangle \ \langle \ell| \exp(-\frac{\beta \mathrm{Le}^2}{2\epsilon}\ell^2) |\ell\rangle \langle \ell|\phi + 2\pi \mathrm{n}\rangle \ \mathrm{e}^{\mathrm{i}(\mathrm{m}-\mathrm{n})\theta}; \tag{16}$$

again, ϕ is the initial value of $(e\tilde{A}^1(q=0))$. Note that we now choose ℓ to be the eigenvalue of the operator $(\epsilon\tilde{E}^1(q=0)/eL)$, hence the factor of ϵ in the denominator of the exponent. Notice that with the modified Lagrangian, it is now $(\epsilon\tilde{E}^1(q=0)/eL)$ which is conjugate to $(e\tilde{A}^1(q=0))$. Therefore,

$$\langle \phi + 2\pi m|\ell\rangle \ = \exp(i(\phi + 2\pi m)\ell) \tag{17}$$

remain unchanged.

Now we can follow through the same calculation, realizing that *it is ℓ that is quantized.* The ground state electric field, following the same argument, should instead be

$$E = -\frac{\theta e}{2\pi\epsilon}, \ -\pi < \theta < \pi. \tag{18}$$

This matches the situation with open ends. The ground state electric field is thus screened as well with periodic boundary conditions and does not take an universal value.

On the other hand, one should also be able to start from vacuum, and understand the screening as a dynamical effect. In the last section, we have found that θ shifts by 2π as we shift the electronic wavefunction by a lattice period. It is thus intuitive to think, that the electrons will shift a little bit, responding to the electric field generated from the θ-term, and make θ smaller. Here we are going to show that this intuitive picture gives precisely the same effect as above.

From the point of view of the charges, θ is the Berry's phase when the system slowly transit from its ground state to another state which is related by a large gauge transform. In the adiabatic limit, we derive that the phase is just the topological index. However, since the θ-term in turn predicts that there in a finite electric field in the ground state, the procedure is actually far from the adiabatic limit, and there can be some extra dynamical phases.

Instead of calculating the dynamical phases in detail, let us switch and suppose we already have the effective theory, with some parameter θ and ϵ. From the effective theory point of view, the accumulated phase in the presence of a finite field is just the first derivative of the electronic action with respect to the electric field. This gives

$$\theta_{\mathrm{Berry}} = \theta + \frac{2\pi}{e}(\epsilon - 1)E. \tag{19}$$

We then proceed with the quantization of the gauge field in vacuum with this modified θ_{Berry}. We get

$$E = -\frac{\theta_{\mathrm{Berry}} e}{2\pi} = -\frac{\theta e}{2\pi} - (\epsilon - 1)E, \tag{20}$$

and we recover the same result as Eq. (18). This calculation matches our intuition that the wave function can adjust itself a little bit (a compromise between a rigid shift and the ionic potential, characterized by the dielectric constant ϵ) to reduce the electric field.

We have to note that the second treatment does not work at finite temperature, as witnessed by the different quantization of the electric field in the two methods. At finite temperature, the electric field fluctuates from the average value. Once the electric field fluctuates around, it would be wrong to identify the contribution from the dielectric constant as a phase, instead of an energy. Nevertheless, one can still expect that treating it as a phase should give correct ground state properties at zero temperature. Physically this is because in the ground state the partition function is dominated by the states with the average electric field. When one calculates the phase accumulated when the gauge winding increases with a fixed electric field, there is no real distinction between the contribution from the geometric Berry's phase and the dynamical phase.

IV. SUMMARY

In this report, we clarified two issues about the ground state electric field in 1D topological insulators.

We showed that in a unit-cell doubled system, it is possible for two states related by a lattice translation, to have a different "topological index" characterizing the electronic band structure. It is still a topological index in the sense that we cannot smoothly change from one state to another without breaking the discrete symmetry (in the SSH model, the inversion symmetry.) However, since the translation of ions also changes the Berry's phase, the two states are physically equivalent. With the ions placed properly, there will be no θ-term in the effective theory, and no ground state electric field. For a tight-binding model without unit-cell doubling and when the electron orbitals are always tied to to the ions, such as the topological insulator in 1D defined under charge conjugation, the topological index of the electronic band does give a ground state electric field, and the topological state and the trivial state are intrinsically different.

We also showed that, unlike our previous comment, the electric field is not perfectly quantized in a system without boundaries. The screening effect, can be either viewed as a change of the quantization of the static electric field in the presence of the dielectric constant, or as a shift of θ in the presence of the field it generates.

We thank C. Kane for pointing out the issues in the SSH model and the fruitful discussion. We acknowledge the support of NSF under grant DMR 1104498.

[1] Kuang-Ting Chen and Patrick A. Lee, Phys. Rev. B **83**, 125119 (2011).
[2] W. P. Su, J. R. Schrieffer, A. J. Heeger, Phys. Rev. B **22**, 2099-2111 (1980).
[3] J. Zak, Phys. Rev. Lett. **62**, 2747 (1989).
[4] R. D. King-Smith and D. Vanderbilt, Phys. Rev. B **47**, 1651 (1993).