I. REFLECTION PROTECTED ATOMIC INSULATORS FROM BAND THEORY

We begin by providing a very general reason that shows why reflection symmetry protects the distinction between the two atomic insulators discussed in the previous lecture. In $k$-space, both $k = 0$ and $k = \pi/a$ are reflection-invariant points. Thus the Bloch functions at either $k$-point must be an eigenfunction of the reflection operator $\Pi$ with eigenvalue $\pm 1$. Let us explicitly find these eigenvalues for the particular Hamiltonian studied previously. The single particle Hamiltonian at a general $k$-point is

$$H(k) = (t_1 + t_2 \cos(ka))\sigma^x - t_2 \sin(ka)\sigma^y$$

Thus we have $H(k = 0) = (t_1 + t_2)\sigma^x$.

Denoting the eigenvector as $\chi(k)$, we have

$$\chi_{\pm}(k = 0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

We are interested in the $\Pi$ eigenvalues which we denote $s_0^\pm$ for these $k = 0$ states. As $\Pi$ acts as $\sigma^x$, it follows that

$$s_0^\pm = \pm 1$$

On the other hand $H(k = \pi) = (t_1 - t_2)\sigma^x$. Now if $t_1 > t_2$, we have

$$\chi_{\pm}(ka = \pi) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$$

while if $t_2 > t_1$, then

$$\chi_{\pm}(k = 0) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \mp 1 \end{pmatrix}$$

Defining the $\Pi$ eigenvalues through $\Pi\chi_{\pm}(ka = \pi) = s_{\pi}^\pm \chi_{\pm}(ka = \pi)$, we have

$$s_{\pi}^\pm = \pm 1 \quad t_1 > t_2$$

$$= \pm 1, \quad t_2 > t_1$$
This for \( t_1 > t_2 \), the reflection eigenvalues at \( k = 0 \) and \( ka = \pi \) are matched with each other while for \( t_2 > t_1 \), they are mismatched with each other. This is a sharp distinction between the two limits which ensures that there is no path within the space of reflection symmetric free fermion Hamiltonians that can connect the two atomic insulating ground states without the band gap closing.

II. RELATION TO QUANTIZED BERRY PHASES

Consider the Bloch functions \( \chi_{k-} \) of, say, the lower band. Associated with the \( k \)-space gauge freedom \( \chi_{k-} \rightarrow e^{i\theta_k} \chi_{k-} \), we can define a \( k \)-space gauge connection

\[
a_-(k) = -i\chi_{k-}^\dagger \frac{d}{dk} \chi_{k-} = -i\langle k - | \frac{d}{dk} | k - \rangle
\]

Clearly under the gauge transformation,

\[
a_-(k) \rightarrow a_-(k) + \frac{d\theta_k}{dk}
\]

In 1d the Brillouin zone is a circle, and periodicity of \( \chi_{k-} \) requires that

\[
\theta_{k + \frac{\pi}{a}} = \theta_k + 2\pi n
\]

Now consider the quantity

\[
\Phi_- = \oint dk a_-(k)
\]

Under the gauge transformation,

\[
\Phi_- \rightarrow \Phi_- + 2\pi n
\]

Thus \( e^{i\Phi_-} \) is completely gauge invariant. For the single particle Hamiltonian \( H(k) \) parametrized by \( k \), \( \Phi_- \) is the Berry phase accumulated as \( k \) is varied adiabatically around the Brillouin zone.

Physically \( \Phi_- \) is related to the bulk electric polarization in this system. Given a band \(|k\rangle\) and some Wannier states \(|R\rangle\), define the Wannier centers \( \bar{r} \) through

\[
\bar{r} - R = \langle R| r - R | R \rangle
\]

\[
= \int dr |w_R(r)|^2 (r - R)
\]

This quantity directly determines the bulk polarization per unit length of the crystal:

\[
P = -\frac{e(\bar{r} - R)}{a} = -\frac{ie}{2\pi} \oint dk \langle k | \frac{d}{dk} | k \rangle
\]
(\(-e\) is the electron charge). Thus \(P\) is directly proportional to the Berry phase of the band: \(P = \frac{e\Phi}{2\pi}\). A 2\(\pi\) shift of the Berry phase shifts \(P\) by \(e\). This simply corresponds to shifting all the electrons by a lattice constant, and does not change the state at all. Thus \(P\) and \(P + ne\) describe the same physical state.

Note that under reflection \(P \rightarrow -P\). For reflection to be a symmetry, we must thus have

\[-P \equiv P + ne\]  

We thus have the general result that in any reflection symmetric 1\(d\) insulator,

\[
P/e = 0 \mod Z, \text{ or } P/e = 1/2 \mod Z \tag{17}
\]

Thus reflection symmetric 1\(d\) insulators come in (at least) two distinct varieties distinguished by whether \(P/e\) is an integer, or shifted from an integer by 1/2.

Let us now return to the SSH model, and determine the Berry phase of the occupied lower band. We first note that due to the reflection symmetry

\[
\sigma^x H(-k) \sigma^x = H(k) \tag{18}
\]

This implies that if \(\chi_{\pm}(k)\) is an eigenvector of \(H(k)\), then \(\sigma^x \chi_{\pm}(k)\) is an eigenvector of \(H(-k)\). As there is an unique eigenstate for each \(k\) within a single band, we write

\[
\sigma^x \chi_-(k) = e^{-i\alpha(k)} \chi_-(k) \tag{19}
\]

As \(\Pi^2 = 1\), we have that

\[
e^{i(\alpha(k) + \alpha(-k))} = 1 \tag{20}
\]

The Berry phase can now be calculated.

\[
\Phi_- = -i \int_{\pi/a}^{\pi/a} \frac{d}{dk} \chi_-(k) \frac{d}{dk} \chi_-(k)
\]

\[
= -i \left( \int_{-\pi/a}^{0} dk + \int_{0}^{\pi/a} dk \right) \chi_-(k) \frac{d}{dk} \chi_-(k)
\]

\[
= -i \int_{0}^{\pi/a} dk \left( -\chi_-(-k) \frac{d}{dk} \chi_-(k) + \chi_-(k) \frac{d}{dk} \chi_-(k) \right)
\]

\[
= -i \int_{0}^{\pi/a} dk \left( -\chi_-(-k) e^{-i\alpha(k)} \frac{d}{dk} (e^{i\alpha(k)} \chi_-(k)) + \chi_-(k) \frac{d}{dk} \chi_-(k) \right)
\]

\[
= -i \int_{0}^{\pi/a} \frac{d\alpha(k)}{dk}
\]

\[
= \alpha(0) - \alpha(\pi/a) \tag{21}
\]
Note that \( e^{i\alpha(0)} = s_0^- \) and \( e^{i\alpha(\pi/a)} = s_\pi^- \) are the reflection eigenvalues at the high symmetry points introduced earlier. This we have our final result

\[
e^{i\Phi_-} = s_0^- s_\pi^-
\]

We learn that if the reflection eigenvalues at \( k = 0 \) and \( k = \pi/a \) are matched then \( \Phi_- = 0 \mod 2\pi \) while if they are mismatched then \( \Phi_- = \pi \mod 2\pi \). Thus we have established a direct connection between the previous discussion of the distinction between the two atomic insulators (in terms of reflection eigenvalues at high symmetry points) and the present discussion in terms of the polarization.

### III. COMMENTS

1. *Stability to interactions*

The different points of view from which we have discussed the sharp distinction between the two atomic insulators in the SSH model each have their advantages. The most physical but also the most powerful is the distinction in terms of the polarization. Phrasing the distinction in terms of polarization is so general that it even applies in the presence of electron-electron interactions. The polarization of course determines the response of the system to a probe external electromagnetic field. Our discussion can be viewed in terms of restrictions placed by reflection symmetry on the electromagnetic response of a 1d crystalline insulator. This point of view also has a generalization to higher dimensions in discussions of other symmetry protected phases.

The points of view in terms of the quantized Berry phase or in terms of reflection eigenvalues at high symmetry points are both specific to free fermion models. Within the scope of such models, they also have useful generalizations to higher dimensional band structures.

2. *Quantum phase transition*

In the SSH model, the phase transition between the two distinct atomic insulators happens at \( t_1 = t_2 \equiv t \). The band gap closes continuously as this point of the phase diagram is approached from either phase. This is a continuous quantum phase transition (often referred to as a quantum critical point). Notice that the distinction between the two phases can (of course) not be captured by the concept of a spontaneously broken symmetry. Thus there is
no notion of a Landau order parameter for this phase transition. At this quantum critical point, the single particle Hamiltonian can be written

$$H(k) = t ((1 + \cos(ka))\sigma^x - \sin(ka)\sigma^y)$$ (23)

The band touching happens at $ka = \pi$. Writing $k = \pi/a + q$ (with $|q| \ll \pi/a$), and linearizing in $q$ gives

$$H(q) \approx tqa\sigma^y$$ (24)

The corresponding many body Hamiltonian can be written

$$\mathcal{H}_{QCP} = L \int \frac{dq}{2\pi} \tilde{c}_q^\dagger (tqa\sigma^y)\tilde{c}_q$$ (25)

This is the Hamiltonian of a massless Dirac fermion in 1d with a Dirac velocity $v = ta$. $L$ is the length of the system. We have left implicit a high momentum cut-off in defining the $q$-integral. Near the critical point there will be universal singularities in physical quantities that can be calculated by taking the cut-off to infinity. We can define a real space continuum Dirac field $\Psi(x)$ through

$$\tilde{c}(q) = \frac{1}{\sqrt{L}} \int dx e^{-iqx} \Psi(x)$$ (26)

Then

$$\mathcal{H}_{QCP} = \int dx \Psi^\dagger \left( -iv\sigma^y \frac{d}{dx} + m\sigma^x \right) \Psi(x)$$ (27)

If we are close to but not quite at the critical point, and we write $t_1 = t + \delta, t_2 = t - \delta$, then the low energy continuum Hamiltonian is readily seen to become

$$\mathcal{H} = \int dx \Psi^\dagger \left( -iv\sigma^y \frac{d}{dx} + m\sigma^x \right) \Psi(x)$$ (28)

where the Dirac ‘mass’ $m = 2\delta$. This massive Dirac Hamiltonian can be used to determine all the universal critical singularities.

3. **Quantum criticality beyond band theory**

(This comment is for the more advanced students). A most interesting phenomenon happens when we consider adding weak short-ranged electron-electron interactions. A discussed above the distinction between the two phases persists. What happens at the phase transition? This can be addressed by considering the effect of such interactions on the massless Dirac fermion theory. It is known that weak short range interactions lead to a fixed line (in the
renormalization group sense) parametrized by the interaction strength. The critical point then becomes a non-Fermi liquid where the electron quasiparticle has been destroyed. In the interacting system then, the electron quasiparticle is well-defined in either of the two phases. Nevertheless, the quasiparticle weight vanishes upon approaching the critical point, and we end up with a non-fermi liquid quantum critical point!