Lecture 19/11 (I.27a)

MODERN THEORY OF ELECTRIC POLARIZATION (CONT'D)

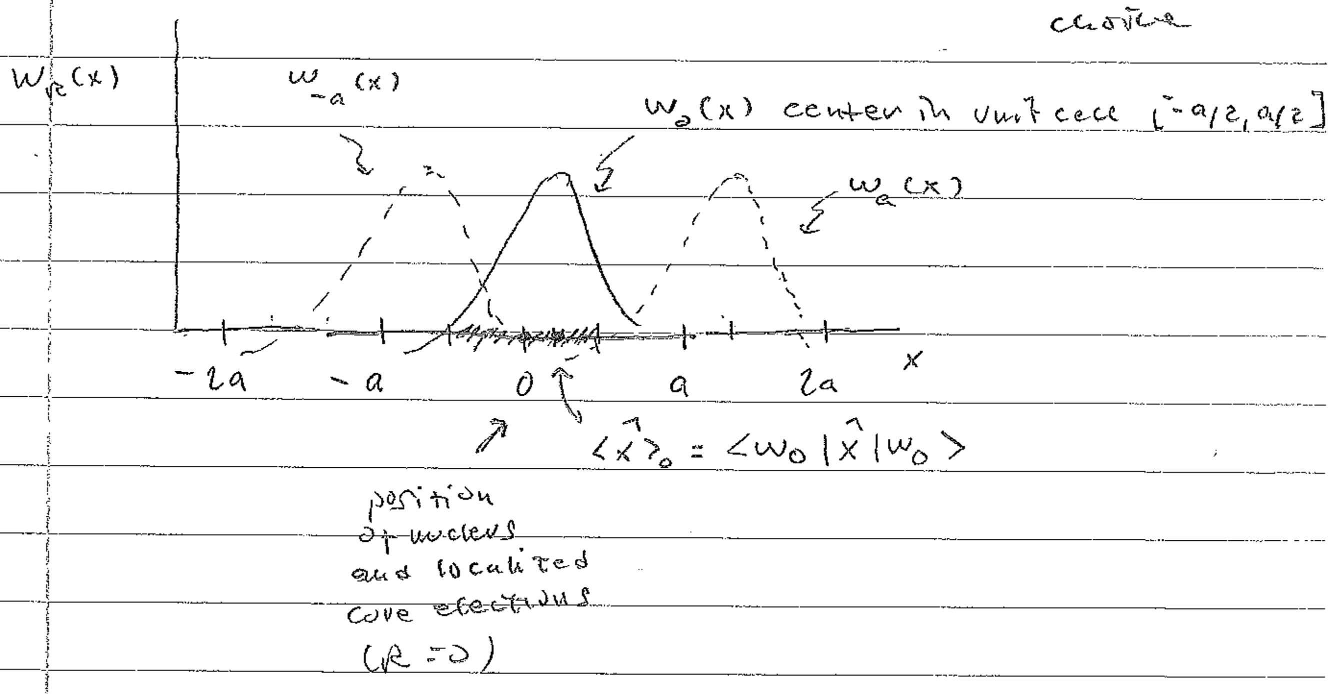
After a review of elementary electron structure, I introduced the notion of WANNIER STATES in my last lecture, and now we'll see how we can use them to calculate the electric polarization of an insulator, tying it to a Berry phase.

ELECTRIC POLARIZATION

$$\vec{P} = -e\frac{\vec{d}}{V_{cell}}, \quad \vec{d} = \langle \hat{\vec{r}} \rangle_0$$

expectation value of valence electron position ~~in a unit cell with $\vec{R}=0$~~

convenient choice



as in the picture on the previous page!

(I.22b

Let's do the analysis in 1D ($\vec{r} = x$, $\vec{R} = R$) and look at a single filled band (suppressing the band index "n")

Note: single-particle analysis!

$$\langle x | w_R \rangle = w_R(x) \overset{(I.42)}{=} \frac{1}{2\pi} \oint_{BZ} e^{-ikR} \psi_k(x)\, dk$$

$$= \frac{1}{2\pi} \oint_{BZ} e^{ik(x-R)} u_k(x)\, dk \qquad (I.46)$$

Consider the unit cell labelled by $R = 0$, $x \in [-a/2, a/2]$

$$\langle \hat{x} \rangle_0 = \langle w_0 | \underbrace{\hat{x} | w_0 \rangle} = \text{peak of Wannier function in unit cell labelled by } R=0 \qquad (I.47)$$

HW: Fill out the missing steps!

$$\hat{x} | w_0 \rangle = \frac{1}{2\pi} \oint_{BZ} \hat{x} \underbrace{e^{ikx} | u_k \rangle}_{*} dk = \frac{1}{2\pi} \oint_{BZ} x\, e^{ikx} | u_k \rangle dk$$

$$= \frac{1}{2\pi} \int_{BZ} (-i\partial_k e^{ikx}) | u_k \rangle dk$$

PARTIAL INTEGRATION
$$= \frac{1}{2\pi} \underbrace{e^{ikx} | u_k \rangle \Big|_0^{2\pi}}_{=0} + \frac{1}{2\pi} \int_0^{2\pi} e^{ikx}\, \underline{i\partial_k | u_k \rangle} dk \qquad (I.48)$$

using that $u_{k=2\pi}(x) = e^{-2\pi i x} u_{k=0}(x)$ from the periodic boundary condition on $\psi_k(x)$: $\psi_{k=2\pi}(x) = \psi_{k=0}(x)$

It follows from (I.48) that

$$\langle \hat{x} \rangle_0 = \langle w_0 | \hat{x} | w_0 \rangle = \frac{1}{2\pi} \oint_{BZ} \underbrace{\langle u_k | i\partial_k | u_k \rangle}_{A(k)} dk$$

BERRY PHASE!
$$= \frac{\Phi}{2\pi} \qquad (I.49)$$

* Here I make a short cut, using that $U_k(x) = \langle x | u_k \rangle = e^{-ikx} \psi_k(x)$
$= e^{-ikx} \langle x | \psi_k \rangle = \langle x | e^{-ikx} | \psi_k \rangle \Rightarrow$ "$| u_k \rangle = e^{-ikx} | \psi_k \rangle$"
OK as an intermediate step

Putting things together: (I.49) together with the expression for the polarization, $\vec{P} = -e\frac{\vec{d}}{V_{cell}} = e\frac{\langle w_0|\hat{x}|w_0\rangle}{V_{cell}}$, we conclude that in 1D ($V_{cell} = a = 1$):

$$\boxed{P = -e\frac{\phi}{2\pi}} \quad \text{(I.50)}$$

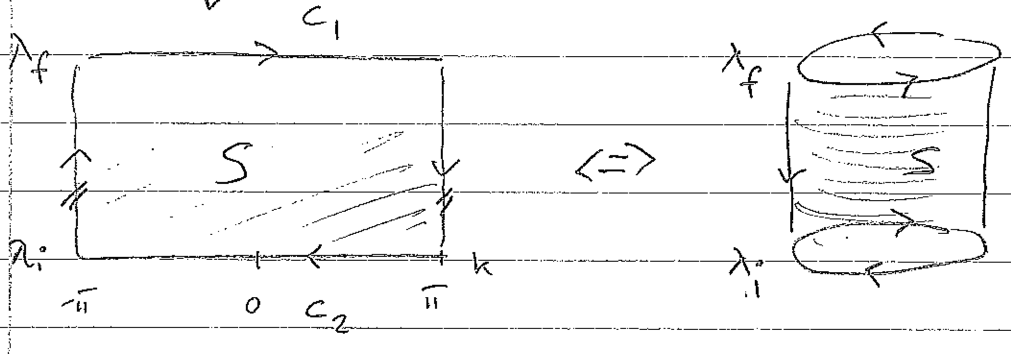
$\phi \leftarrow$ Berry phase!

But ϕ is not gauge invariant! Hence, by (I.50), P is not an observable! However, the change of P is an observable. Basic idea: Introduce a parameter λ (μ, p, ...) and consider the change ΔP of P as λ changes from λ_i to λ_f:

$$\Delta P = P_{\lambda_f} - P_{\lambda_i} = \frac{e}{2\pi}\left(\oint_{C_1} - \oint_{C_2}\right) \underbrace{\mathcal{A}_k}_{\text{Berry connection}} dk$$

$$\overset{\text{Stokes}}{=} \frac{e}{2\pi}\int_S \underbrace{\mathcal{F}_k}_{\text{Berry curvature}} dk\, d\lambda \quad \text{(I.51)}$$

$\Downarrow$



ΔP calculated using $\mathcal{F}_k$ is well defined since $\mathcal{F}_k$ is gauge invariant. Note that S is an open surface. Hence, we can't use the Chern theorem. In other words, no reason to believe that ΔP is quantized.

Why all this fuss about electric polarization in a course on topology in physics?! (I.29

ANSWER: By adding certain symmetry constraints to the model we are studying, we can make ΔP quantized! And not only that, the quantization of ΔP signals a TOPOLOGICAL PHASE, more precisely a

TOPOLOGICAL PHASES IN NATURE

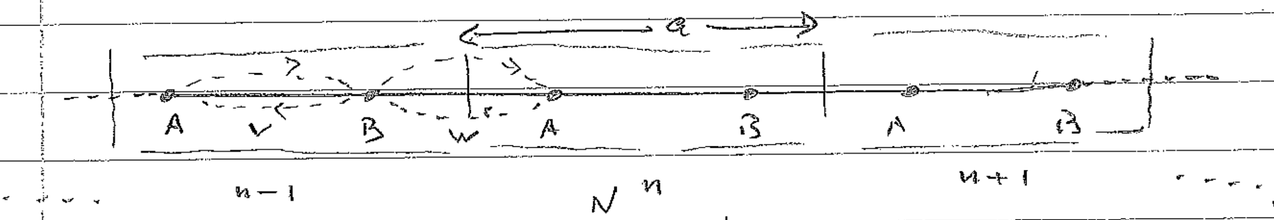
SYMMETRY PROTECTED TOPOLOGICAL PHASES.

TOPOLOGICALLY ORDERED PHASES

CASE STUDY: SU-SCHRIEFFER-HEEGER (SSH) MODEL

SSH model, introduced in the 1970s to study conjugated polymer chains. (Nobel prize in Chemistry 2000 for discovery of conducting polymers)
Today, the spinless version of the model is the very simplest model that supports a topological phase ("hydrogen atom of topological quantum matter").

$v, w \in \mathbb{R}$



HAMILTONIAN: $$H = \sum_{n=1}^{N}\left(v\, c^\dagger_{A,n} c_{B,n} + w\, c^\dagger_{A,n+1} c_{B,n} + \text{H.c.}\right)$$ (I.52)

$v = t + \delta t$ $\quad$ $w = t - \delta t$

DIMERIZED HOPPING AMPLITUDES FROM "PEIERLS INSTABILITY"

Discuss!

$$\begin{cases} a_k = \frac{1}{\sqrt{N}} \sum_n e^{-ik\overbrace{na}^{\text{"}x\text{"}}} c_{A,n} \\ b_k = \frac{1}{\sqrt{N}} \sum_n e^{-ikna} c_{B,n} \end{cases}$$

$$\Rightarrow \quad H = v \sum_{k\in[-\pi/a,\, \pi/a]} \left(a_k^\dagger b_k + b_k^\dagger a_k\right) + w \sum_k \left(e^{ika} a_k^\dagger b_k + e^{-ika} b_k^\dagger a_k\right)$$ (I.53)

Introducing $\Psi_k = \begin{pmatrix} a_k \\ b_k \end{pmatrix}$, we can write (I.53) on the form

$$H = \sum_k \Psi_k^+ \underbrace{\Big((v + w\cos(ka))\sigma_x + w\sin(ka)\sigma_y\Big)}_{H(k) = \begin{pmatrix} 0 & d_x - id_y \\ d_x + id_y & 0 \end{pmatrix}} \Psi_k \qquad (I.54)$$

SINGLE-PARTICLE "BLOCH HAMILTONIAN"

Note: Any 2x2 Hamiltonian matrix can be expanded in the basis of Pauli matrices: $H(k) = \vec{d}(k) \cdot \vec{\sigma}$, $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. SSH model: $d_x(k) = v + w\cos(ka)$, $d_y(k) = w\sin(ka)$, $d_z(k) = 0$

$H(k)$ can be easily diagonalized by using $H(k)^2 = |\vec{d}(k)|^2 \mathbb{1}$.

$$\Rightarrow \quad \underset{\text{lower band}}{\overset{\text{upper band}}{E_\pm(k)}} = \pm|\vec{d}(k)| = \pm\sqrt{v^2 + w^2 + 2vw\cos ka} \qquad (I.55a)$$

PICTURE: SLIDE! 21/11

$$|u_\pm(k)\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} \pm e^{-i\varphi(k)} \\ 1 \end{pmatrix}, \quad \varphi(k) = \arctan\left(\frac{d_y(k)}{d_x(k)}\right) \qquad (I.55b)$$

The Bloch Hamiltonian is cell-periodic
$\Rightarrow$ (eigenstates) are the cell-periodic Bloch states $|u_\pm(k)\rangle$

Consider the two cases $v > w$, $v < w$ $\Rightarrow$ well-separated bands $\pm$ ("gapped spectrum" $\Rightarrow$ band insulator when the $-$ band is completely filled). For these cases the Berry phases for the $+$ and $-$ bands are well defined (no band degeneracies). Let's calculate the BERRY PHASE Φ_- for the $-$ band! (The Berry phase obtained by integrating over a 1D BZ is called a ZAK PHASE (after the Israeli physicist Joshua Zak) $\longrightarrow$

$$= \oint_{BZ} \dots$$

put $a=1$ in (I.55b)

$$\Phi_- = \int_{-\pi}^{\pi} \langle u_-(k) | i\partial_k | u_-(k) \rangle$$

$$= i \int_{-\pi}^{\pi} \langle u_-(k) | \nabla_{\vec{d}} | u_-(k) \rangle \cdot \frac{d\vec{d}}{dk} dk$$

$\vec{d}(d_x(k), d_y(k), 0)$

$$= i \oint_{\Gamma} \langle u_-(k) | \nabla_{\vec{d}} | u_-(k) \rangle \cdot d\vec{d}$$

Γ ← closed loop traversed by $\vec{d}(k)$ ~~as k sweeps through the BZ~~

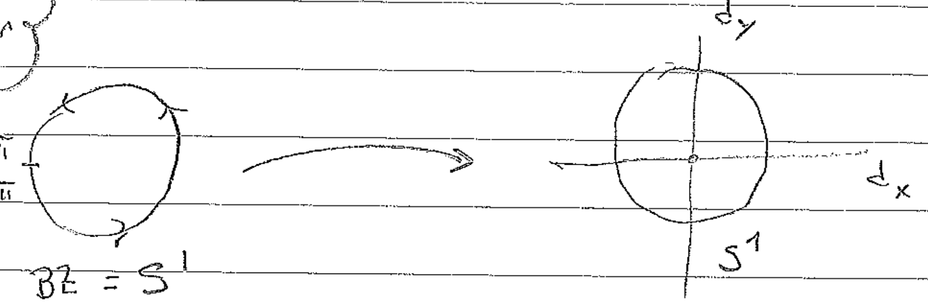
$$= \begin{cases} 0 & \text{if } v > w \\ -\pi & \text{if } v < w \end{cases} \qquad (I.56)$$

$$\text{Define } \mathcal{N} = -\frac{\Phi}{\pi} = \begin{cases} 0 & \text{if } v > w \\ 1 & \text{if } v < w \end{cases} \qquad (I.57)$$

WINDING NUMBER

TOPOLOGICAL INVARIANT CHARACTERIZING THE MAPPING $S^1 \rightarrow S^1$

Study behavior of $\vec{d}(k)$ as we sweep the BZ!



1D BZ = S^1

"How many times does the image of the 1D BZ wrap around the origin in "Hamiltonian space"?"

parameterized by $d_x(k), d_y(k)$

FIGURE: SLIDE! 21/11

$\mathcal{N} = 0$ TRIVIAL INSULATOR

$\mathcal{N} = 1$ TOPOLOGICAL INSULATOR