Lecture 14/11

REVIEW OF ELECTRON STRUCTURE THEORY

As I announced Tuesday, we shall now apply "Berryology" to the Brillouin torus of electrons in a crystal, laying the ground work for topological band theory.

But first: A comment on my Tuesday discussion of adiabatic evolution (reviewing Michael Berry's famous paper from 1984). The Ansatz as I originally wrote it

$$|\Psi(t)\rangle = c(t)\, e^{-i\beta(t)} \underbrace{|u(t)\rangle}_{=|u(\lambda(t))\rangle}$$

$|u(\lambda(t))\rangle$ = instantaneous t eigenstate

is correct! Slippery notation, leading to some confusion. Think about it this way: In a time-independent problem we would have

$$\beta(t) = \frac{1}{\hbar}\int_0^t E_n(t')\,dt' = \frac{1}{\hbar}E_n t \quad \text{(time-independent case)}$$

$$|\Psi(t)\rangle = e^{-i\beta(t)}\,|u(0)\rangle$$

$|u(0)\rangle$ = instantaneous eigenstate at $t=0$ and for all times incl. at t arbitrary!

In the time-dependent problem we replace $|u(0)\rangle$ by the instantaneous eigenstate at t, i.e. $|u(\lambda(t))\rangle$ and hang on an additional phase $c(t)$. The correctness of this procedure is proven by showing that $|\Psi(t)\rangle$ solves the time-dependent Schrödinger equation (with proper choice of $c(t)$ $(= e^{i\phi(t)})$).

ϕ: BERRY PHASE!

Let's first recall some basics of ELECTRONS IN A CRYSTAL !

We consider a crystal with lattice vectors $\vec{R}_{\vec{\ell}} = \ell_1 \vec{a}_1 + \ell_2 \vec{a}_2 + \ell_3 \vec{a}_3$

condition for discrete translational invariance

Consider a Hamiltonian H, $[H, \bar{T}_{\vec{a}_j}] = 0$, where $\bar{T}_{\vec{a}_j}$ is the translation operator that shifts the system by $\vec{a}_j$, $j = 1,2,3$

$\bar{T}_{\vec{a}_j}$ is unitary $\rightarrow$ its eigenvalues can be written as $e^{-i d\ell_j}$, where $d\ell_j$ is a phase angle. The Bloch theorem follows directly

$$H|\Psi_{n\vec{d\ell}}\rangle = \bar{E}_{n\vec{d\ell}} |\Psi_{n\vec{d\ell}}\rangle \qquad (\bar{I}.24)$$

with $\vec{d\ell} = (d\ell_1, d\ell_2, d\ell_3)$, and n a "band index" that counts states of the same $\vec{d\ell}$ in order of increasing energy. The states $|\Psi_{n\vec{d\ell}}\rangle$ have the property that $\bar{T}_{\vec{a}_j} |\Psi_{n\vec{d\ell}}\rangle = e^{-i d\ell_j} |\Psi_{n\vec{d\ell}}\rangle$ or, equivalently, (in coordinate representation, generalizing to arbitrary lattice translations),

$$\Psi_{n\vec{d\ell}}(\vec{r} + \vec{R}_{\vec{\ell}}) = e^{i\vec{d\ell}\cdot\vec{\ell}} \Psi_{n\vec{d\ell}}(\vec{r}) \qquad (\bar{I}.25)$$

We can write Bloch's theorem on a more familiar form by introducing the reciprocal lattice spanned by vectors $\vec{b}_j$ that are dual to $\vec{a}_j$: $\vec{a}_i \cdot \vec{b}_j = 2\pi \delta_{ij}$ * The dual to $\vec{R}_{\vec{\ell}}$ is usually denoted by $\vec{G}_{\vec{m}} = m_1 \vec{b}_1 + m_2 \vec{b}_2 + m_3 \vec{b}_3$.

Defining the wave vectors $\vec{k} = \frac{d\ell_1}{2\pi}\vec{b}_1 + \frac{d\ell_2}{2\pi}\vec{b}_2 + \frac{d\ell_3}{2\pi}\vec{b}_3$, Bloch's theorem becomes (with the states labelled by $\vec{k}$ instead of $\vec{d\ell}$)

$$H|\Psi_{n\vec{k}}\rangle = \bar{E}_{n\vec{k}} |\Psi_{n\vec{k}}\rangle \qquad (\bar{I}.26)$$

$\vec{R} = \vec{R}_{\vec{\ell}}$ suppressed

with $\langle \vec{r} + \vec{R} | \Psi_{n\vec{k}} \rangle = \Psi_{n\vec{k}}(\vec{r} + \vec{R}) = e^{i\vec{k}\cdot\vec{R}} \Psi_{n\vec{k}}(\vec{r}) \qquad (\bar{I}.27$

$\hat{n} \not\parallel \vec{a}_1 \times \vec{a}_2$

* 2D : $\vec{b}_1 = 2\pi (\vec{a}_2 \times \hat{n}) / |\vec{a}_1 \times \vec{a}_2|$ and similarly for $\vec{b}_2$

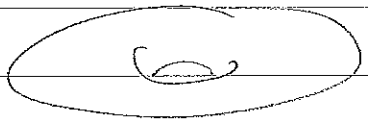
3D : $\vec{b}_1 = 2\pi (\vec{a}_2 \times \vec{a}_3) / |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$ and similarly for $\vec{b}_2, \vec{b}_3$

By periodicity (cf. (I.27)),

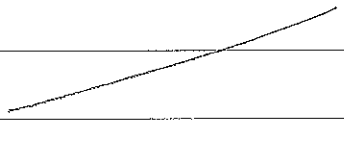
$\vec{k}$ and $\vec{k}+\vec{G}$ are duplicate labels for the same state, for any $\vec{G}$ $\Rightarrow$ a single unit cell in reciprocal space is enough to label each state once and only once. We call this unitcell the BRILLOUIN ZONE, with boundary condition

$$|\psi_{n,\vec{k}+\vec{G}}\rangle = |\psi_{n,\vec{k}}\rangle \qquad (I.28)$$

By (I.28), the BZ is a closed manifold without a boundary in 2) (3) topologically equivalent to a 2- (3-) torus



$S^1 \times S^1$ = Cartesian product of two circles



$S^1 \times S^1 \times S^1$

(hard to draw !)

The Bloch functions $\psi_{n\vec{k}}(\vec{r})$ in (I.27) satisfy twisted boundary conditions on the primitive cell of the direct (original) crystal lattice. Much simpler to work with the cell-periodic Bloch functions

$$u_{n\vec{k}}(\vec{r}) = e^{-i\vec{k}\cdot\vec{r}}\psi_{n\vec{k}}(\vec{r}) \qquad (I.29)$$

which satisfy

("direct") lattice vector

$$u_{n\vec{k}}(\vec{r}+\vec{R}) = u_{n\vec{k}}(\vec{r}) \qquad (I.30)$$

It follows from (I.28) that

$$u_{n,\vec{k}+\vec{G}}(\vec{r}) = e^{-i\vec{G}\cdot\vec{r}}\, u_{n\vec{k}}(\vec{r}) \qquad (I.31)$$

Nice property of $u_{n\vec{k}}(\vec{r})$: $\nabla_{\vec{k}} u_{n\vec{k}}(\vec{r})$ well-defined periodic functions belonging to the same tangent space. *

Compare with the nasty behavior of $\nabla_{\vec{k}} \psi_{n\vec{k}}(\vec{r}) =$

$$= e^{i\vec{k}\cdot\vec{r}}\left(\nabla_{\vec{k}} u_{n\vec{k}}(\vec{r}) + i\vec{r}\, u_{n\vec{k}}(\vec{r})\right)$$

blows up with the distance from $\vec{r}=0$

* As we shall see, this property is crucial for defining a Berry phase with the BZ as parameter space!

Given the cell-periodic Bloch functions we can define a BLOCH HAMILTONIAN

$$H(\vec{k}) = e^{-i\vec{k}\cdot\vec{r}}\, H\, e^{i\vec{k}\cdot\vec{r}} \qquad (I.32)$$

such that

$$H(\vec{k})\,|u_{n\vec{k}}\rangle = E_{n\vec{k}}\,|u_{n\vec{k}}\rangle \qquad (I.33)$$

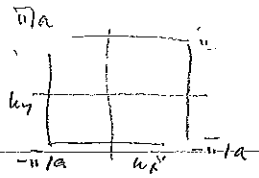
We are now ready to specialize our discussion of Berry phases, connections, curvatures, and fluxes to the case where the parameters $\lambda = (\lambda_1, \lambda_2, \ldots)$ are wave vector components k_i labelling cell-periodic Bloch states $|u_{n\vec{k}}\rangle$ of band n in the Brillouin zone (BZ), with $\vec{k} = k_1, k_2, k_3$.

Look at the discretized Berry phase

* $\langle u_k | \psi_{k+\Delta k}\rangle = \int_{-\infty}^{\infty} dx\, e^{i\Delta k x} u_k^*(x) u_k(x) = 0 \Rightarrow \phi = -\ln(\ldots) \to -\infty$

"washes out" the contribution from $u_k^*(x) u_k(x)$

periodic with the unit cell

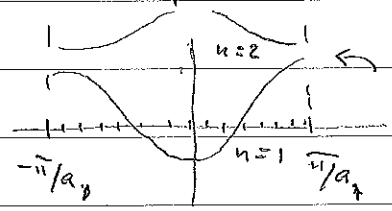


← simple square lattice BZ

Let's look at 2D.

Assuming that we have well-separated bands in the BZ

(BAND INSULATOR)



← gapped everywhere

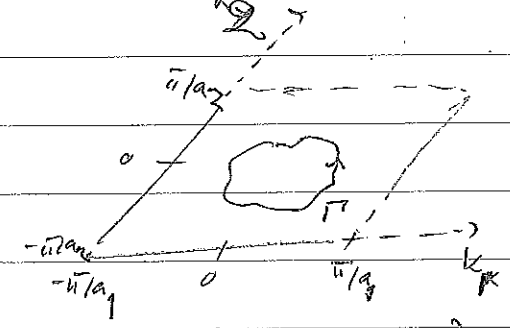
$N = N_1 \times N_2 \times N_3$ primitive cells

$\vec{k} = \left(n_1/N_1\right)\vec{b}_1 + \left(n_2/N_2\right)\vec{b}_2 + \left(n_3/N_3\right)\vec{b}_3$, $n_j = 0, \ldots, N_j$, $j = 1, 2, 3$

$\sum_{\vec{k}} \rightarrow \frac{V_{cell}}{(2\pi)^3}\int d^3k$

We can then define a Berry phase for each band n:

$$\Phi_n = \oint_\Gamma \vec{A}_n(\vec{k}) \cdot d\vec{k} \qquad (I.34)$$



with Berry connection $\vec{A}_n(\vec{k}) = \left(A_{nk_x}(\vec{k}), A_{nk_y}(\vec{k})\right)$

$$A_{n\mu}(\vec{k}) = \langle u_{n\vec{k}} | i\partial_\mu | u_{n\vec{k}} \rangle \quad , \mu = k_x, k_y \qquad (I.35)$$

$\partial_\mu \equiv \partial_{k_\mu}$

In vector form:

$$\vec{A}_n(\vec{k}) = \langle u_{n\vec{k}} | i\nabla_{\vec{k}} | u_{n\vec{k}} \rangle \qquad (I.36)$$

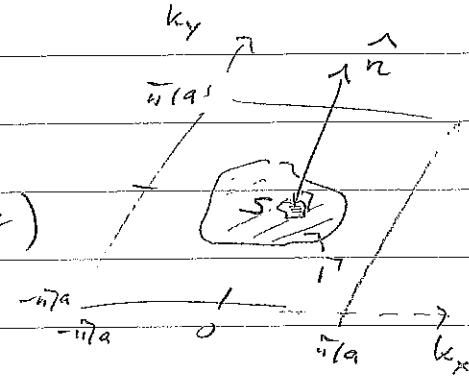
Corresponding Berry curvature

$$\vec{F}_n(\vec{k}) = \nabla_{\vec{k}} \times \vec{A}_n(\vec{k}) \qquad (I.37)$$

yielding a Berry flux

$$\Phi_n = \int_S \vec{F}_n(\vec{k}) \cdot d\vec{S} \qquad (I.38)$$

$d\vec{S} = dS\hat{n}$



As we have seen, in 2D the BZ = torus (closed manifold) and by choosing S = BZ in (I.38) we obtain the Chern number for the entire band labelled by n:

$$\frac{1}{2\pi}\int_{BZ} \vec{F}_n(\vec{k}) \cdot d\vec{S} = C_n \qquad (I.39)$$

As before, the Berry connection $\vec{A}_n(\vec{k})$ is gauge dependant:

$$|u_{n\vec{k}}\rangle \to |\tilde{u}_{n\vec{k}}\rangle = e^{-i\beta(\vec{k})}|u_n(\vec{k})\rangle$$

$$\tilde{A}_n(k) = A_n(\vec{k}) + \nabla_{\vec{k}}\beta(k) \qquad (I.40)$$

while the curvature $\vec{F}_n(\vec{k})$ (and hence the Chern number) is fully gauge-invariant.

It is easy to show that (i) if the crystal has inversion symmetry, then $\vec{F}_n(\vec{k}) = \vec{F}_n(-\vec{k})$; and (ii) time-reversal invariance implies that $\vec{F}_n(\vec{k}) = -\vec{F}_n(-\vec{k})$; and (iii) the Chern number vanishes for time-reversal invariant systems. (A "historic"—exploded! aside: the subject of topological quantum matter took off when Charlie Kane & Gene Mele in 2005 showed that one can define another type of topological invariant which does not vanish for time-reversal invariant systems: the "Z_2 index".)

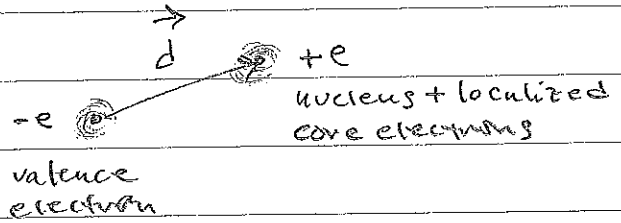
HW

MODERN THEORY OF POLARIZATION FROM THE BERRY PHASE.

A very interesting and instructive application of Berry phase calculations for electronic states in the BZ of a crystal is provided by the "modern theory of electric polarization". *

The basic problem here is how to calculate the electric polarization $\vec{P}$ (= density of electric dipole moments) of an insulator. Consider a monatomic crystal. For this case, the obvious choice would be to define

$$\vec{P} = e \frac{\vec{d}}{V_{cell}} \quad \text{(unit cell volume)} \qquad (I.41)$$



However, the valence electron is delocalized / "smeared out", occupying an extended Bloch state => "center of negative charge" is ill defined. A possible way out is to change basis from the extended Bloch states to localized WANNIER STATES.

* R. Resta, Ferroelectrics 136, 51 (1992)
R.D. King-Smith and D. Vanderbilt, Phys. Rev. B47, 1651 (1993)

$\psi_{n,k=-\pi/a}(x) = \psi_{n,k=\pi/a}(x)$

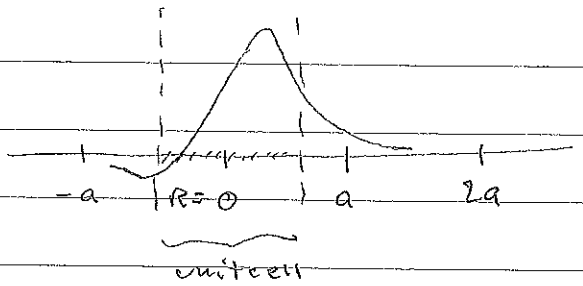
To define the Wannier states, we assume a smooth and periodic gauge for the Bloch functions $|\psi_{n\vec{k}}\rangle$. We can then Fourier transform to obtain

$$|w_{n\vec{R}}\rangle = \frac{V_{cell}}{(2\pi)^3}\int_{BZ} e^{-i\vec{k}\cdot\vec{R}}\,|\psi_{n\vec{k}}\rangle\, d^3k \qquad (I.42)^*$$

(V_{cell}: unit cell volume)

$$|\psi_{n\vec{k}}\rangle = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}}\,|w_{n\vec{R}}\rangle$$

$\langle \vec{r}\,|w_{n\vec{R}}\rangle = w_{n\vec{R}}(\vec{r})$ is a localized function centered near $\vec{R}$:



One can show that the Wannier functions form an ON basis

$$\langle w_{n\vec{R}}|w_{n'\vec{R}'}\rangle = \delta_{nn'}\delta_{\vec{R}\vec{R}'} \qquad (I.43)$$

using the normalization

$$\int_{V_{cell}} |\psi_{n\vec{k}}(\vec{r})|^2 d^3r = \int_{V_{cell}} |u_{n\vec{k}}(\vec{r})|^2 d^3r = \langle u_{n\vec{k}}|u_{n\vec{k}}\rangle = 1 \qquad (I.44)$$

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* NOTE $\langle \vec{r}\,|w_{n\vec{R}}\rangle = w_{n\vec{R}}(\vec{r}) = \frac{V_{cell}}{(2\pi)^3}\int_{BZ} e^{-i\vec{k}\cdot\vec{R}}\underbrace{\langle \vec{r}\,|\psi_{n\vec{k}}\rangle}_{\psi_{n\vec{k}}(\vec{r})} d^3k$

decays rapidly with $\vec{R}$ for fixed $\vec{r}$, i.e. $w_{n\vec{R}}(\vec{r}) \to 0$ as $|\vec{r}-\vec{R}| \to \infty$. Equivalent to a rapid decay with $\vec{r}$ for fixed $\vec{R}$.

Important properties of the Wannier functions:

1. Localization: $|w_{n\vec{R}}(\vec{r})| \longrightarrow 0$ for $|\vec{r}-\vec{R}|$ large (I.45a)

2. Translational image: $w_{n\vec{R}}(\vec{r}) = w_{n\vec{0}}(\vec{r}-\vec{R})$ (I.45b)

3. $\{|w_{n\vec{R}}\rangle\}$ form an ON basis (I.45c)

4. $\langle w_{n\vec{0}}|H|w_{n\vec{R}}\rangle = \bar{E}_{n\vec{R}}$ (I.45d)

$\vec{R}$-component of Fourier expansion based on

$$\bar{E}_{n\vec{R}} = \left(V_{cell}/(2\pi)^3\right) \int_{BZ} e^{-i\vec{k}\cdot\vec{R}} \bar{E}_{n\vec{k}}\, d^3k$$