ECE 5390 / MSE 5472, Fall Semester 2017

Quantum Transport in Electron Devices and Novel Materials

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Assignment 5, Solutions

Problem 5.1: The Berry Phase and Chern Numbers

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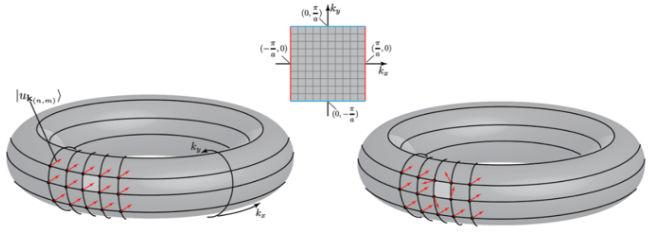


Figure 1: Berry phase and Chern Number.

Consider a discrete grid for the parameter space $\mathbf{k} = (k_x, k_y) = (n, m)$ of a Hamiltonian $\hat{H}(\mathbf{k})$ that has eigenfunctions and eigenvalues given by the Schrodinger equation $\hat{H}(\mathbf{k})|\psi_\mathbf{k}\rangle = E(\mathbf{k})|\psi_\mathbf{k}\rangle$. Now consider the eigenfunctions as vectors in the Hilbert space defined over a 2D parameter space in the form of a 2D Brillouin zone as shown in Figure 1. To prepare for electron transport in a 2D system, we assume that the Brillouin zone is a torus, and the discrete grid (n, m) forms closed cyclic loops in values of (k_x, k_y). Choose the gauge to be $|\psi_\mathbf{k}\rangle \rightarrow e^{i\alpha_\mathbf{k}}|\psi_\mathbf{k}\rangle$, a $\mathbf{k}$-dependent phase factor multiplied by the eigenfunction.

(a) Show that the net phase accumulated in traversing an **open path** on the grid is **not gauge invariant** because it depends on the gauge factors $\alpha_\mathbf{k}$.

(b) Show why the net phase accumulated in traversing **any closed path** on the grid on the torus is **gauge invariant**. This is the Berry phase γ_L around a Loop, defined by

$$e^{i\gamma_L} = \text{Arg}[\langle\psi_{\mathbf{k_1}}|\psi_{\mathbf{k_2}}\rangle \cdot \langle\psi_{\mathbf{k_2}}|\psi_{\mathbf{k_3}}\rangle \cdot \langle\psi_{\mathbf{k_3}}|\psi_{\mathbf{k_4}}\rangle \cdot ... \cdot \langle\psi_{\mathbf{k_N}}|\psi_{\mathbf{k_1}}\rangle]. \tag{1}$$

(c) Show why the closed loop chain of inner products in the discrete form of the Berry phase above becomes a line integral in the limiting continuum case, i.e.

$$\gamma_L = i \oint d\mathbf{k} \cdot \underbrace{\langle\psi_\mathbf{k}|\nabla_\mathbf{k}|\psi_\mathbf{k}\rangle}_{\mathcal{A}_\mathbf{k}}, \tag{2}$$

where ∇ is the gradient operator[1]. Here $\mathcal{A}_\mathbf{k}$ is the Berry connection.

(d) The discrete Berry **flux** F is defined as the sum of the phases around a closed loop or a plaquette, say around the lightly shaded rectangle in Figure 1 moving in a counterclockwise direction. Show why the net Berry flux through a closed loop satisfies the Stokes theorem - like relation to the Berry phase:

$$e^{i\sum_\mathbf{k} F_\mathbf{k}} = e^{i\gamma_L} \leftrightarrow e^{i\int d\mathbf{S_k}\cdot\mathbf{F_k}} = e^{i\oint d\mathbf{k}\cdot\langle\psi_\mathbf{k}|\nabla_\mathbf{k}|\psi_\mathbf{k}\rangle}. \tag{3}$$

what is different from the Stokes theorem? Show how the discrete Berry flux leads to the Berry curvature $\mathcal{B}_\mathbf{k}$ in the continuum case defined as

$$\mathcal{B}_\mathbf{k} = \nabla_\mathbf{k} \times \mathcal{A}_\mathbf{k} \leftrightarrow \oint d\mathbf{k} \cdot \mathcal{A}_\mathbf{k} = \int d\mathbf{S_k} \cdot \underbrace{\nabla_\mathbf{k} \times \mathcal{A}_\mathbf{k}}_{\mathcal{B}_\mathbf{k}}. \tag{4}$$

(e) Argue why the sum of the Berry fluxes for any closed orientable surface must follow the relation

$$\prod_\mathbf{k} e^{iF_\mathbf{k}} = e^0 = 1 = e^{i2\pi\times Q} \leftrightarrow \oint d\mathbf{S_k} \cdot \mathcal{B}_\mathbf{k} = 2\pi Q \tag{5}$$

where $Q = \frac{\sum_\mathbf{k} F_\mathbf{k}}{2\pi}$ is an integer. This integer is the Chern number.

(f) Argue why the Chern number counts how many **vortices** of the eigenvectors are present in the parameter surface, for example the torus of Figure 1.

Solution: [By Ian Briggs, 2017]

1). $\vec{k} = (k_x, k_y) = (n, m)$ $\quad \hat{H}(k)|\psi_k\rangle = E(k)|\psi_k\rangle$

gauge: $|\psi_k\rangle \to e^{i\alpha_k}|\psi_k\rangle$

a). $\psi_{1\to 2\to 3\to\cdots\to n} = \langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\cdots\langle\psi_{n-1}|\psi_n\rangle$

$= \langle\psi_1|e^{-i\alpha_1}e^{i\alpha_2}|\psi_2\rangle\langle\psi_2|e^{-i\alpha_2}e^{i\alpha_3}|\psi_3\rangle\cdots$
$\langle\psi_{n-1}|e^{-i\alpha_{n-1}}e^{i\alpha_n}|\psi_n\rangle$

$= e^{i(\alpha_2-\alpha_1)}e^{i(\alpha_3-\alpha_2)}\cdots e^{i(\alpha_n-\alpha_{n-1})}\langle\psi_1|\psi_2\rangle\langle\psi_2|\psi_3\rangle\cdots\langle\psi_n|\psi_1\rangle$

$\gamma = \arg\{\psi_{1\to 2\to 3\to\cdots\to n}\} = \alpha_n - \alpha_1$

→ not gauge invariant

b). $\mathrm{Arg}[\langle\psi_1|e^{-i\alpha_1}e^{i\alpha_2}|\psi_2\rangle\langle\psi_2|e^{-i\alpha_2}e^{i\alpha_3}|\psi_3\rangle\cdots\langle\psi_n|e^{-i\alpha_n}e^{i\alpha_1}|\psi_1\rangle]$

$= (\alpha_2-\alpha_1) + (\alpha_3-\alpha_2) + \cdots + (\alpha_1-\alpha_n)$

→ all gauge terms cancel in summation

→ closed loop is gauge invariant

c). $\gamma_L = \sum_{n,m} F_{n,m}$

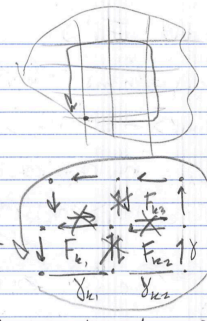
$F_{n,m} = \mathrm{phase}\{\langle\psi_n|\psi_m\rangle\}$

for continuum case: $e^{-i\Delta\gamma} = \dfrac{\langle\psi(k)|\psi(k+dk)\rangle}{|\langle\psi(k)|\psi(k+dk)\rangle|}$

$\Delta\gamma = i\langle\psi(k)|\nabla_k|\psi(k)\rangle dk$

$\gamma_L = \lim_{dk\to 0}\sum\Delta\gamma = i\oint dk\langle\psi_k|\nabla_k|\psi_k\rangle$

d). $A_k = \langle\psi_k|\nabla_k|\psi_k\rangle$



→ only border elements of fluxes do not cancel

$\gamma_L = \sum_k \gamma_k = \sum F_k = \int dS_k F_k = \oint dk\langle\psi_k|\nabla_k|\psi_k\rangle$

in continuous case, according to Stokes thm

$\oint d\vec{k}\cdot A_k = \int dS_k\cdot(\underbrace{\nabla_k \times A_k}_{B_k})$

e). $|\psi_k\rangle = e^{i\alpha_k}|\psi_{k_0}\rangle$

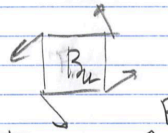
$|\psi_k\rangle \to e^{i\gamma_L}|\psi_k\rangle$

in order to satisfy boundary conditions around the closed loop γ_L must be an integer multiple of 2π

$\prod e^{iF_k} = e^{i\sum F_k} = 1$

$\gamma_L = \oint d\vec{k}\cdot A_k = \int dS_k \nabla\times A_k = 2\pi Q$

if each vortex in phase contributes 2π in phase to the closed integral



$\gamma_L = \int dS_k B_k = \int dS_k \nabla\times A_k$

B_k is nonzero only for presence of vortex → Q counts the # of vortices in the integration area

Problem 5.2: Berry Phase and Berry Curvature

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We discussed the origin of the Berry phase in quantum mechanics by constructing a state $|\psi_n(\mathbf{k})\rangle = e^{i\gamma_n(t)}e^{-\frac{i}{\hbar}\int_0^t E_n dt'}|n(\mathbf{k})\rangle$. Here $\mathbf{k}(t)$ is a *parameter* on which the state depends adiabatically: for example, the wavevector for electrons in a crystal. We can vary the wavevector $\mathbf{k}(t)$ with time, by applying a magnetic (or electric) field. We let the Hamiltonian operator $\hat{H}$ and the time-dependent energy operator $i\hbar\frac{\partial}{\partial t}$ act on this state separately, and then projected the new state at time t back to $\langle n(k(t))|$. Time-dependent Schrodinger equation demands that they be *exactly the same*, for all possible quantum states. Then one must have $\gamma_n(t) = \int_C d\mathbf{k}\cdot\mathcal{A}$, where $\mathcal{A} = i\langle n|\frac{\partial}{\partial\mathbf{k}}|n\rangle$ is an effective vector potential, analogous to the magnetic vector potential, and C is the path in $\mathbf{k}$ space traversed in the process of time evolution. If one makes a gauge transformation of the state $|\psi_n(\mathbf{k})\rangle \to e^{i\theta(\mathbf{k})}|\psi_n(\mathbf{k})\rangle$, the effective vector potential changes to $\mathcal{A} \to \mathcal{A} - \frac{\partial\theta(\mathbf{k})}{\partial\mathbf{k}}$. Since all physical observables must be gauge-invariant, one could dismiss the above phase in part (a) as unphysical. However, Berry argued that if we *close* the path, then $\boxed{\gamma_n = \oint_C d\mathbf{k}\cdot\mathcal{A}}$ becomes gauge-invariant: verify his assertion. This is the Berry phase, and $\mathcal{A} = i\langle n|\frac{\partial}{\partial\mathbf{k}}|n\rangle$ is the Berry vector potential.

(a) Electrons in 2D graphene have a Dirac-cone bandstructure whose eigenstates near the Dirac points in $\mathbf{k}$-space may be represented as $|\mathcal{K}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{2}}\begin{pmatrix}1\\ e^{-i\theta}\end{pmatrix}$ and $|\mathcal{K}'\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{2}}\begin{pmatrix}1\\ e^{+i\theta}\end{pmatrix}$, where $\tan\theta = k_y/k_x$, and the states are defined on the (k,θ) plane. By integrating along a circular loop centered at the Dirac point, show that the Berry phases of the states are $\gamma_{\mathcal{K}} = +\pi$ and $\gamma_{\mathcal{K}} = -\pi$.

(b) In analogy to the relation between the magnetic vector potential and the magnetic field, we defined the Berry curvature as $\mathcal{B}_{\mathbf{k}} = \nabla\times\mathcal{A}(\mathbf{k})$ via the Stoke's theorem $\gamma_n = \oint_C d\mathbf{k}\cdot\mathcal{A} = \int_S d\mathbf{S}\cdot(\nabla\times\mathcal{A})$. Here S is the *surface* enclosed in the parameter space by the closed loop C. Show that the Berry curvature can be written as a sum over eigenstates:

$$\mathcal{B}_{\mu\nu}(\mathbf{k}) = i[\langle\frac{\partial u_n}{\partial k_\mu}|\frac{\partial u_n}{\partial k_\nu}\rangle - \langle\frac{\partial u_n}{\partial k_\nu}|\frac{\partial u_n}{\partial k_\mu}\rangle] = i\sum_{n'\neq n}\frac{\langle n|\partial_{k_\mu}\hat{H}|n'\rangle\langle n'|\partial_{k_\nu}\hat{H}|n\rangle - \langle n|\partial_{k_\nu}\hat{H}|n'\rangle\langle n'|\partial_{k_\mu}\hat{H}|n\rangle}{(E_n - E_{n'})^2} \tag{6}$$

(c) Show that the Berry curvature of Graphene is zero everywhere *except* at the Dirac points, where it diverges. Even though it diverges, it has a finite integral: what is the integral of the Berry curvature around the Dirac points $\mathcal{K}$ and $\mathcal{K}'$?

Solutions: [Parts a & b By Sam Bader, 2015 and c by Ian Briggs, 2017]

If we make a gauge transformation $|\psi(k)\rangle \to e^{i\theta(k)}|\psi(k)\rangle$, then $\mathcal{A}$ transforms as $\mathcal{A} \to \mathcal{A} - \nabla_k \theta(k)$. If we integrate $\mathcal{A}$ along a closed path C which starts (arbitrarily) from k_0 and loops back to k_0,

$$\gamma_n = \oint_C dk \cdot \mathcal{A}$$

then γ_n transforms as

$$\gamma_n \to \gamma_n - \oint_C dk \cdot \nabla_k \theta(k)$$

For this transformation to be a well-defined (ie single-valued) function, $\theta(k)$ can, at most, be multi-valued modulo 2π. So the right-term is an integer times 2π. Then $e^{i\gamma_n}$ is unchanged by this transformation.

a)

First, calculate the Berry potential near the Dirac point $\mathcal{K}$

$$\begin{aligned}
\mathcal{A}_\mathcal{K} &= i\langle \mathcal{K}|\nabla_{\vec{k}}|\mathcal{K}\rangle \\
&= i\frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}1 & e^{i\theta}\end{pmatrix}\nabla_{\vec{k}}\left[\frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}1\\ e^{-i\theta}\end{pmatrix}\right] \\
&= i\frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}1 & e^{i\theta}\end{pmatrix}\left[\frac{i\vec{r}e^{i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}1\\ e^{-i\theta}\end{pmatrix} + \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}0\\ -ik\hat{\theta}e^{-i\theta}\end{pmatrix}\right] \\
&= i\frac{e^{-i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}1 & e^{i\theta}\end{pmatrix}\left[\frac{i\vec{r}e^{i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}1\\ e^{-i\theta}\end{pmatrix} + \frac{e^{i\vec{k}\cdot\vec{r}}}{\sqrt{2}}\begin{pmatrix}0\\ -(i\hat{\theta}/k)e^{-i\theta}\end{pmatrix}\right] \\
&= -\vec{r} + \frac{\hat{\theta}}{2k}
\end{aligned}$$

And by tracing the negative sign on the θ through the above, we see that, for the other Dirac point, $A_{\mathcal{K}'} = -\vec{r} - \frac{\hat{\theta}}{2k}$.

Now integrate around a Dirac point.

$$\gamma_\mathcal{K} = \oint_C d\vec{k} \cdot \mathcal{A}_\mathcal{K} = \int_0^{2\pi} k d\hat{\theta} \cdot \left(-\vec{r} + \frac{\hat{\theta}}{2k}\right)$$

The first term integrates to zero, since $\hat{\theta}$ rotates all the way around the circle of integration while $\vec{r}$ stays constant. The second term is aligned for the whole integral, so

$$\gamma_\mathcal{K} = \pi$$

And similarly, including the extra negative on the other Dirac point,

$$\gamma_{\mathcal{K}'} = -\pi$$

b)

$$A = i\langle n|\nabla_k|n\rangle$$

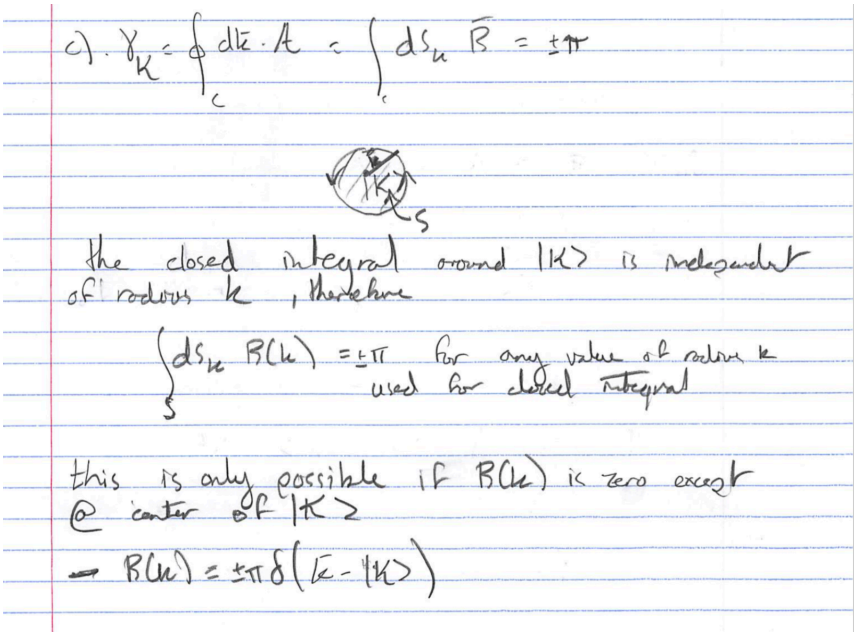
$$\Omega_{n,\mu\nu} = \epsilon_{\delta\mu\nu}[\nabla_k \times \mathcal{A}]_\delta = i\left(\partial_{k_\mu}\langle n|\partial_{k_\nu}n\rangle - \partial_{k_\nu}\langle n|\partial_{k_\mu}n\rangle\right) = i\left(\langle\partial_{k_\mu}n|\partial_{k_\nu}n\rangle - \langle\partial_{k_\nu}n|\partial_{k_\mu}n\rangle\right)$$

Using standard first-order perturbation theory,

$$|\partial_{k_\nu}n\rangle = \sum_{n'\neq n}\frac{\langle n'|\partial_{k_\nu}H|n\rangle}{E_n - E_{n'}}|n'\rangle$$

Plugging this in above and using the orthogonality of the $|n'\rangle$ states to kill one summation immediately yields the required result

$$\Omega_{n,\mu\nu} = \sum_{n' \neq n} \frac{\langle n|\partial_{k_\mu} H|n'\rangle\langle n'|\partial_{k_\nu} H|n\rangle - \langle n|\partial_{k_\nu} H|n'\rangle\langle n'|\partial_{k_\mu} H|n\rangle}{(E_n - E_{n'})^2}$$



Problem 5.3: Quantum Hall Effect and Chern Number

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We have discussed in class that the transverse conductance $\rho_{xy} = n\frac{e^2}{h}$ in the integer quantum Hall insulator state of a 2D electron gas is quantized to parts-per-billion precision for 2DEGs across various material families such as Silicon MOSFETs, III-V 2DEGs, oxide 2DEGs, graphene, etc. An explanation for the precision of the quantization is offered by the Berry phase which requires that the integer n of quantization is exactly the Chern number of the Berry phase. This connection was made by Thouless and co-workers[2]. In this problem, you will work through the arguments.

(a) Outline why the velocity of a quantum state of charge q and bandstructure $E(\mathbf{k})$ when the Berry phase is taken into account is given by

$$\mathbf{v} = \frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k}) + \frac{q}{\hbar}\mathbf{E} \times \mathcal{B}(\mathbf{k}), \tag{7}$$

where $\mathcal{B}(\mathbf{k})$ is the Berry curvature of the band and $\mathbf{E}$ is the electric field. Note that the velocity in the second term is perpendicular to the external electric field.

(b) Use the standard quantum mechanical expression for the current density in the n$^{\text{th}}$ 2D band

$$\mathbf{J} = q\sum_n \int \frac{d^2\mathbf{k}}{(2\pi)^2}\mathbf{v}_n(\mathbf{k}) f(\mathbf{k}), \tag{8}$$

to argue why the first standard velocity term $\frac{1}{\hbar}\nabla_{\mathbf{k}} E(\mathbf{k})$ gives zero net current if the band is *completely filled*. This is the situation when the magnetic field has formed Landau levels and the Fermi energy lies in the gap between 2 Landau levels, $\sigma_{xx} \to 0$ and $\sigma_{xy} = n\frac{e^2}{h}$, which we have referred to as the quantum-Hall insulator states.

(c) Now show why for such filled Landau levels, the transverse conductance J_x/E_y is given by the second velocity term $\frac{q}{\hbar}\mathbf{E} \times \mathcal{B}(\mathbf{k})$, and the conductance with $q = -e$ is

$$\sigma_{xy} = \frac{J_x}{E_y} = \frac{e^2}{h}\sum_n \Big(\underbrace{\frac{\int d^2\mathbf{k} \cdot \mathcal{B}^{\mathbf{n}}_{\mathbf{k}}}{2\pi}}_{Q_n = \text{Chern Number}} \Big) = \frac{e^2}{h} \times \text{integer}, \tag{9}$$

i.e., the Hall conductance is quantized. The quantization is precise to parts per billion because the Chern number for each band is mathematically constrained to be an integer.

[2] This connection was established in: Thouless, Kohmoto, Nightingale, den Nijs (TKNN), Phys. Rev. Lett. **49** 405 (1882). Note that they do not call the Berry phase or curvature by name in this paper, because Berry's paper came out 2 years after the TKNN paper!

Solution: [By Sam Bader, 2015 and Andrei Isichenko, 2017]

First, I'll derive the expression for group velocity, for a Bloch state k, starting from a generic Hamiltonian

$$E(k) = \langle \psi_{nk} | H | \psi_{nk} \rangle = \langle \psi_{nk} | \frac{p^2}{2m} + V(x) | \psi_{nk} \rangle$$

I'd like to take the k-derivative of both sides, but, with the k-dependance inside of the Bloch states, that leads to some mathematically dubious things. (For one, the $\psi_k(x)$ is not a pointwise continuous function of k because the e^{ikx} allows you to always choose a larger x to make $\psi_k(x)$ vary faster with k... in fact, in the infinite volume limit, ψ_k are orthogonal even for arbitrarily closely spaced k.) But we can gather exponential k-dependence into a parametric Hamiltonian $H_k = e^{-ikx} H e^{ikx}$ one the space of strictly periodic $u_{nk}(x)$ functions, after which our operations will be well-defined mathematically.

$$E(k) = \langle u_{nk} | H_k | u_{nk} \rangle = \langle u_{nk} | e^{-ikx} \left(\frac{p^2}{2m} + V(x) \right) e^{ikx} | u_{nk} \rangle$$

This simplifies to

$$\langle u_{nk} | H_k | u_{nk} \rangle = \langle u_{nk} | \frac{(p + \hbar k)^2}{2m} + V(x) | u_{nk} \rangle$$

Now we differentiate (making use of the Hellman-Feynman theorem)

$$\langle u_{nk} | \nabla_k H_k | u_{nk} \rangle = \langle u_{nk} | \frac{\hbar (p + \hbar k)}{m} | u_{nk} \rangle$$

Now move the exponential dependance back into the states:

$$\langle u_{nk} | \nabla_k H_k | u_{nk} \rangle = \langle u_{nk} | e^{-ikx} \frac{\hbar p}{m} e^{ikx} | u_{nk} \rangle$$

$$\langle u_{nk} | \nabla_k H_k | u_{nk} \rangle = \langle \psi_{nk} | \frac{\hbar p}{m} | \psi_{nk} \rangle = \hbar v_g$$

Thus we can write the group velocity as

$$v_g = \frac{1}{\hbar} \langle u_{nk} | \nabla_k H_k | u_{nk} \rangle$$

If we now consider the Hamiltonian subject to an electric field, which we will include via the vector potential so as not to break the translational invariance of the potential energy term,

$$H = \frac{(p - qEt)^2}{2m} + V(x)$$

And treat the electric field as a perturbation, then we find, to first-order

$$|u_{nk}\rangle = |u_{nk}^{(0)}\rangle - i\hbar \sum_{n \neq n'} \frac{|u_{n'k}^{(0)}\rangle \langle u_{n'k}^{(0)} | \partial_t u_{nk}^{(0)} \rangle}{E_{nk}^{(0)} - E_{n'k}^{(0)}}$$

Plugging that into our above expression for group velocity, and making use of another first-order perturbation theory result $\langle u_{n'k}^{(0)} | \nabla_k H_k | u_{nk}^{(0)} \rangle = (E_{nk} - E_{n'k}) \langle \nabla_k u_{n'k}^{(0)} | u_{nk}^{(0)} \rangle$, we get

$$v_g = \nabla_k E(k) - i \left(\langle \nabla_k u_{nk}^{(0)} | \partial_t u_{nk}^{(0)} \rangle - \langle \partial_t u_{nk}^{(0)} | \nabla_k u_{nk}^{(0)} \rangle \right)$$

wherein we recognize a "Berry curvature" in $k - t$ space:

$$v_g = \nabla_k E(k) - \Omega_{n,kt}$$

In order to relate this to the more familiar k-space Berry curvature Ω_n, we recall that the effect of t is just advancing k and a change of variables is possible

$$v_g = \nabla_k E(k) + \frac{e}{\hbar} \Omega_n \times \vec{E}$$

In this form, it's much easier to see the relation to the Quantum Hall Effect. If one integrates over the whole filled band, then the first term will vanish, but the second provides a current perpendicular to the electric field. And that term is proportial to the the band-integrated Berry phase, a quantized value, which explains why the quantum hall effect is so robust.

(b, c)

3b $\vec{J} = q \sum_n \int \frac{d^2\vec{u}}{(2\pi)^2} v_n(\vec{u})\, f(\vec{u})$ current density in the n^{th} 2D band.

If the band is completely filled, ← CB empty, VB filled

Let's park our E_F between the bands - i.e. so it doesn't touch a band and so that no states are removed from V.B.

$$\vec{J}_{2D} = q \int_{-k_{F,source}}^{k_{F,source}} \frac{d^2u}{(2\pi)^2} v_n f(u) \qquad J_{2D} = \int_{-k_{F,drain}}^{k_{F,drain}} \frac{d^2u}{(2\pi)^2} v_n(u) f(u)$$

There are no states $|u| > |u_{max\ VB}|$, so these integrals become the same → In other words, (7) there is no net current.

3c For such filled Landau levels, the transverse conductance $\sigma_{xy} = J_x/E_y$ comes from the anomalous velocity term.

$$\vec{v}_{anomalous} = \frac{q}{\hbar} \vec{E} \times \vec{B}(\vec{u})$$

$$\vec{J}_{2D} = \frac{q g_s g_v}{L^2} \sum \vec{v}_{anom}(\vec{u})\, f(\vec{u})$$

$$= \frac{q g_s g_v}{L^2} \int\int \frac{d^2u}{(2\pi)^2} \frac{q}{\hbar} \vec{E} \times \vec{B}(\vec{u})\, f(\vec{u}) \quad (f \to 1:\ \text{assume band is completely filled})$$

$\vec{E} = E_y \hat{y}$

$$\vec{J} = \frac{q^2 g_s g_v}{4\pi^2 \hbar} E_y\, \hat{y} \times \int\int d^2k\ \vec{B}(\vec{u})$$

take $\hat{x}$ component

$$\frac{J_x}{E_y} = \frac{q^2 g_s g_v}{4\pi^2 \hbar} \int\int d^2k\ \hat{x} \cdot \left(\hat{y} \times \vec{B}(\vec{u})\right) = \frac{q^2 g_s g_v}{4\pi^2 \hbar} \int\int d^2u\ B_z$$

(other components integrate to 0)

$$\frac{J_x}{E_y} = \frac{q^2 g_s g_v}{4\pi^2 \hbar} \oint dS_u \cdot B_z \hat{z}$$

(via flux through flat surface in u-space; Chern number Q)

$$\sigma_{xy} = \boxed{\frac{q^2}{h} Q} \rightarrow \text{the Hall conductance is quantized.}$$

Problem 5.4) The Anomalous Hall Effect

When Edwin Hall discovered the Hall effect in 1879, he observed that *ferromagnetic* metals such as Nickel exhibited a rather strange Hall voltage in addition to the standard linear term in B that is present in non-magnetic metals. In fact ferromagnets can exhibit a Hall-voltage in the absence of an external B field! This phenomenon is known as the Anomalous Hall effect, and an *intrinsic* origin of this effect is explained by the Berry phase. In this problem, we use a toy model to understand this effect[3].

(a) Show why the transverse conductance of a partially filled band in $d-$dimensions is given by

$$\sigma_{xy} = \frac{e^2}{\hbar}\int \frac{d^d\mathbf{k}}{(2\pi)^d} f(E_\mathbf{k})\mathcal{B}_{k_x,k_y}, \tag{10}$$

where $f(E_\mathbf{k})$ is the occupation function of state $\mathbf{k}$ and $\mathcal{B}$ is the Berry curvature of the band.

(b) Argue the connection of the above to the integer quantum Hall effect, i.e., why for a partially filled band even with a zero Chern number a nonzero anomalous Hall conductivity is provided by the *local* Berry curvature.

(c) A model Hamiltonian for bands in a ferromagnetic metal split by strong spin-orbit interactions is

$$H = \frac{\hbar^2k^2}{2m} + \lambda(\mathbf{k}\times\sigma)\cdot\mathbf{e_z} - \Delta\sigma_z, \tag{11}$$

where $\sigma = (\sigma_x,\sigma_y,\sigma_z)$ are Pauli spin matrices, $\mathbf{e_z}$ is a unit vector in the $z-$sirection, λ is the spin-orbit coupling strength, and Δ is an exchange field. Show that the resulting energy dispersion is $E_\pm = \frac{\hbar^2k^2}{2m} \pm \sqrt{\lambda^2k^2+\Delta^2}$. Make a qualitiative plot of this bandstructure and label all relevant parameters.

(d) Show that the Berry curvature of the two bands are $\mathcal{B}_\pm = \mp\frac{\lambda^2\Delta}{2(\lambda^2k^2+\Delta^2)^{\frac{3}{2}}}$. Using this formula, make a plot of the $T\to 0$ K anomalous Hall conductance $\sigma_{xy}(E_F)$ as a function of the Fermi energy E_F and align it with the bandstructure. Show that the anomalous Hall conductivity reaches a magnitude of $\frac{e^2}{2h}$ inside the window $-\Delta \le E_F \le \Delta$ and drops rapidly outside the window.

[3] Refer to Section III.D of the posted review paper Xiao, Chang and Niu, Rev. Mod. Phy. **82** 1959 (2010) for this problem.

Solution: [By Sayak Ghosh, 2017]

5.4) a) using the expression of velocity,

$$\vec{v} = \frac{1}{\hbar}\nabla_k E(\vec{k}) + \frac{q}{\hbar}\vec{E}\times\vec{B}(\vec{k})$$

Current density,

$$\vec{J} = q\int \frac{d^dk}{(2\pi)^d} f(E_{\vec{k}})\,\vec{v}(\vec{k})$$

for filled bands, because of symmetry of band structure ($f(E_k) = f(E_{-\vec{k}})$, $\vec{v}(\vec{k}) = -\vec{v}(-\vec{k})$),

$\vec{J} = 0$

So, current carried by partially filled band. only 2nd term in $\vec{v}$ can give current perpendicular to Electric field. using this,

$$\sigma_{xy} = \frac{\vec{J}_\perp}{|\vec{E}|} = \frac{q}{|\vec{E}|}\int \frac{d^dk}{(2\pi)^d} f(E_{\vec{k}})\cdot\frac{q}{\hbar}(\vec{E}\times\vec{B})_\perp$$

let $\vec{E}$ be along $\hat{y}$. We want $(\vec{E}\times\vec{B})_x$

$(\vec{E}\times\vec{B})_x = E B_z$. Now, since

$\vec{B} = \vec{\nabla}_k\times\vec{A}_k \Rightarrow B_z = \partial_{k_x}A_{k_y} - \partial_{k_y}A_{k_x}$

$= B_{k_x,k_y}$

$$\therefore \sigma_{xy} = \frac{q^2}{\hbar}\int \frac{d^dk}{(2\pi)^d}\frac{f(E_k)E_y B_{k_x,k_y}}{E_y}$$

$$= \frac{q^2}{\hbar}\int \frac{d^dk}{(2\pi)^d} B_{k_x,k_y} f(E_k)$$

b) Clearly, from above result, if band has zero Chern number, still the integral of B_{k_x,k_y} over partially filled band can be non-zero, giving non-zero Hall conductivity.
So, local Berry curvature provides anomalous Hall conductivity.

c) $H = \frac{\hbar^2k^2}{2m} + \lambda(\vec{k}\times\vec{\sigma})\cdot\hat{z} - \Delta\sigma_z$

$= \frac{\hbar^2k^2}{2m} + \lambda k_x\sigma_y - \lambda k_y\sigma_x - \Delta\sigma_z$

Comparing with our standard form for 2-D Hermitian Hamiltonians,

$h_0 = \frac{\hbar^2k^2}{2m}$, $h_x = -\lambda k_y$, $h_y = \lambda k_x$, $h_z = -\Delta$

Energy eigenvalues,

$$E_\pm(k) = h_0 \pm |\vec{h}| = \frac{\hbar^2 k^2}{2m} \pm \sqrt{\lambda^2 k^2 + \Delta^2}$$

Energy eigenstates,

$$u_\pm = \begin{pmatrix} 1 \\ \frac{h_x + i h_y}{h_z \pm |\vec{h}|} \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{-\lambda(k_y - i k_x)}{\Delta \pm \sqrt{\Delta^2 + \lambda^2 k^2}} \end{pmatrix}$$

d) To calculate Berry curvature,

$$B_\pm(\vec{k}) = i\left[\left\langle \frac{\partial u_\pm}{\partial k_x} \middle| \frac{\partial u_\pm}{\partial k_y} \right\rangle - \left\langle \frac{\partial u_\pm}{\partial k_y} \middle| \frac{\partial u_\pm}{\partial k_x} \right\rangle\right]$$

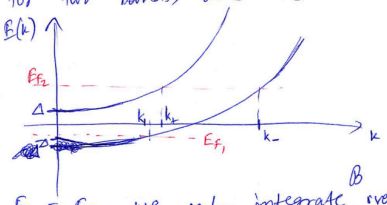
Using $u_\pm$ derived above, and evaluating above expression in Mathematica, gives,

$$B_\pm(\vec{k}) = \mp \frac{\lambda^2 \Delta}{2(\lambda^2 k^2 + \Delta^2)^{3/2}}$$

Using the expression in (a),

$$\sigma_{xy} = \frac{e^2}{\hbar} \int \frac{d^2k}{4\pi^2} f(E_k) B(k_x, k_y)$$

Now, for two bands, looks like



If $E_f = E_{f_1}$, we only integrate B over lower band, all k_x, k_y giving non-zero σ_{xy}.

But if $E_f = E_{f_2}$, we integrate over lower band till k_- and upper band to k_+, and clearly some of the integrals would cancel since B has opposite signs for 2 bands. Thus, if E_f is in range $-\Delta \le E_f \le \Delta$, large σ_{xy} and B falls off rapidly outside this window.

Problem 5.5: Topological Insulators, Winding Numbers, and Berry Phase

Problem 5.5) Topological Insulators, Winding Number, Berry Phase

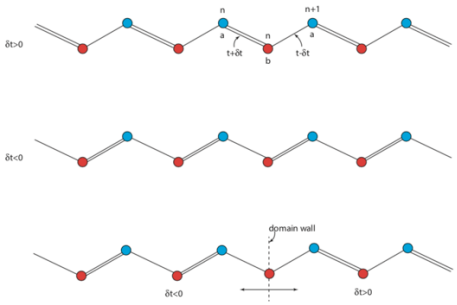


Figure 2: A polyacetylene chain that exhibits a non-trivial topological feature in its bandstructure.

In class, we discussed that *every* 2×2 Hermitian Hamiltonian matrix can be written as

$$H_2 = \begin{pmatrix} h_0(k)+h_z(k) & h_x(k)-ih_y(k) \\ h_x(k)+ih_y(k) & h_0(k)-h_z(k) \end{pmatrix}, \tag{12}$$

and can be decomposed into the form

$$H_2 = h_0(k)I + h_x(k)\sigma_x + h_y(k)\sigma_y + h_z(k)\sigma_z = h_0(k)I + \vec{h}\cdot\vec{\sigma}, \tag{13}$$

where $\vec{h} = [h_x(k), h_y(k), h_z(k)]$, σ's are the Pauli spin matrices, and I is the identity matrix.

(a) By drawing analogy to the Hamiltonian of an electron in a magnetic field and Zeeman splitting, show that the eigenvalues form two bands $E_\pm(k) = h_0(k) \pm |\vec{h}(k)|$, and the gap at k is $E_g(k) = E_+(k) - E_-(k) = 2|\vec{h}(k)|$. Show that the eigenfunctions are not well behaved near points in $k-$space where the *gap closes*. Recall from our discussion of the Dirac monopole that this is a signature of non-trivial Chern-numbers.

(b) We discussed in class that the simplest topologically non-trivial Hamiltonian is for electron transport in the 1D long-chain organic molecule Polyacetylene (see Fig 2) that has alternating single and double bonds between Carbon atoms a and b. Because of the asymmetry in the hopping terms, the tight-binding Hamiltonian is $H = \sum_n \left(\left[(t+\delta t) c^\dagger_{a,n} c_{b,n} + (t-\delta t) c^\dagger_{a,n+1} c_{b,n} \right] + \left[c.c. \right] \right)$ in the occupation number formalism. Show that the resulting $k-$space Hamiltonian is $H = \int \frac{dk}{2\pi} \begin{pmatrix} c^\dagger_{a,k} & c^\dagger_{b,k} \end{pmatrix} \begin{pmatrix} h_0(k)+h_z(k) & h_x(k)-ih_y(k) \\ h_x(k)+ih_y(k) & h_0(k)-h_z(k) \end{pmatrix} \begin{pmatrix} c_{a,k} \\ c_{b,k} \end{pmatrix}$, where $h_x(k) = (t+\delta t) + (t-\delta t)\cos ka$, $h_y(k) = (t-\delta t)\sin ka$, and $h_z(k) = 0$. This is the celebrated "Su-Schrieffer-Heeger" or SSH model.

(c) Assuming $t = 1$ eV, plot the bandstructures for $\delta t = -0.1$ eV, $\delta t = 0.0$ eV, and for $\delta t = +0.1$ eV. What happens as δt goes smoothly through $\delta t = 0$: is there a difference between the states at $\delta t = -0.1$ and $\delta t = +0.1$?

(d) Because $\vec{h}(k) = [h_x(k), h_y(k), h_z(k)]$ may be pictured as an effective magnetic field vector, prove that since $h_z(k) = 0$, as k changes, the tip of the vector $\vec{h}(k)$ *winds around* the origin of the $[h_x(k), h_y(k)]$ plane ZERO times for $\delta t > 0$ but ONE time if $\delta t < 0$.

(d) Show that the Berry phase for $\delta t > 0$ is ZERO, but for $\delta t < 0$ is π. Draw the similarity of this situation with the Dirac monopole problem discussed in class.

(e) If an interface is created between the alternating double and single bonds (see Fig 2), argue that there must be a topologically protected eigenstate at zero energy at the interface. This is the simplest realization of a 'topological insulator'.

Solution: [By Sam Bader, 2015]

a)

The Hamiltonian $H = h_0(k)I + \vec{h}(k) \cdot \vec{\sigma}$ can be viewed a magnetic dipole in a B-field. (To translate, h_0 is just an offset energy, which could be zeroed, and $\vec{h}(k)$ could be interpreted as $\mu\vec{B}$ for this analogy.) Using the standard solution from the Zeeman problem ($E = \pm\mu|B|$), we can immediately write the spectrum for this problem:

$$E = h_0 \pm |\vec{h}(k)|$$

And the eigenvectors are

$$|+\rangle = \begin{pmatrix} e^{-i\phi}\cos(\theta/2) \\ \sin(\theta/2) \end{pmatrix}, \quad |-\rangle = \begin{pmatrix} e^{-i\phi}\sin(\theta/2) \\ -\cos(\theta/2) \end{pmatrix}$$

where θ and ϕ are the spherical-coordinate angles of $\vec{h}(k)$.

At $|\vec{h}(k)| = 0$, these angles become ill-defined. One can approaching the $|\vec{h}(k)| \to 0$ limit from any direction (ie any fixed θ, ϕ), and the eigenvectors will be constant all the way until $|\vec{h}(k)| = 0$, ie $|\pm\rangle$ does not depend on the magnitude of $\vec{h}$, only the direction. So the value of the eigenvectors in the $|\vec{h}(k)| \to 0$ limit depends on which direction you approach from.

b)

Note: to match the notation of the assignment, I will use a to indicate both a basis atom (a vs b) and the unit cell length (eg a is the distance between the any neighboring pair of b atoms or pair of a atoms). I don't think this will cause confusion.

$$H = \sum_n (t+\delta t)c^\dagger_{a,n}c_{b,n} + (t-\delta t)c^\dagger_{a,n+1}c_{b,n} + h.c.$$

Plug in the Fourier transform $c_{a/b,n} = \sum_k e^{iakn}c_{a/b,n}$

$$H = \sum_{nkk'} (t+\delta t)e^{ina(k'-k)}c^\dagger_{a,k}c_{b,k'} + (t-\delta t)e^{ina(k'-k)-iak}c^\dagger_{a,k}c_{b,k'} + h.c.$$

$$H = \sum_{kk'} (t+\delta t)\delta_{k,k'}c^\dagger_{a,k}c_{b,k'} + (t-\delta t)\delta_{k,k'}e^{-iak}c^\dagger_{a,k}c_{b,k'} + h.c.$$

$$H = \sum_k (t+\delta t)c^\dagger_{a,k}c_{b,k} + (t-\delta t)e^{-iak}c^\dagger_{a,k}c_{b,k} + h.c.$$

$$H = \sum_k \left[(t+\delta t) + (t-\delta t)\cos(ak) - i(t-\delta t)\sin(ak)\right] c^\dagger_{a,k}c_{b,k} + h.c.$$

$$H = \begin{pmatrix} c^\dagger_{a,k} & c^\dagger_{b,k} \end{pmatrix} \begin{pmatrix} 0 & (t+\delta t) + (t-\delta t)\cos(ak) - i(t-\delta t)\sin(ak) \\ (t+\delta t) + (t-\delta t)\cos(ak) + i(t-\delta t)\sin(ak) & 0 \end{pmatrix} \begin{pmatrix} c_{a,k} \\ c_{b,k} \end{pmatrix}$$

We can write this as

$$H = \begin{pmatrix} c^\dagger_{a,k} & c^\dagger_{b,k} \end{pmatrix} \begin{pmatrix} h_0(k) + h_z(k) & h_x(k) - ih_y(k) \\ h_x(k) + ih_y(k) & h_0(k) - h_z(k) \end{pmatrix} \begin{pmatrix} c_{a,k} \\ c_{b,k} \end{pmatrix}$$

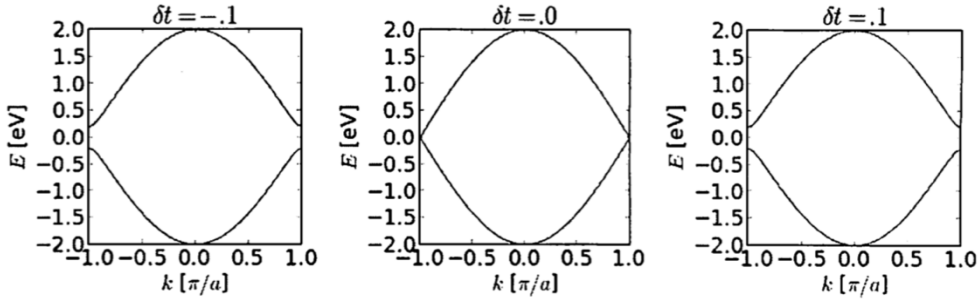
where

$$h_0(k) = 0, \quad h_x(k) = (t+\delta t) + (t-\delta t)\cos(ak), \quad h_y(k) = (t-\delta t)\sin(ak), \quad h_z(k) = 0$$

c)

```
def plotBS(t,dt):
    k=linspace(-pi,pi)
    hx=(t+dt)+(t-dt)*cos(k)
    hy=(t-dt)*sin(k)
    plot(k/pi,sqrt(hx**2+hy**2),'b')
    plot(k/pi,-sqrt(hx**2+hy**2),'b')
    xlabel('$k$ [$\pi/a$]')
    ylabel('$E$ [eV]')

figure(figsize=(12,4))
subplot(131)
plotBS(1,-.1)
title('$\delta t=-.1$')
subplot(132)
plotBS(1,0)
title('$\delta t=.0$')
subplot(133)
plotBS(1,.1)
title('$\delta t=.1$')
tight_layout()
```



The bandstructure is the same for positive and negative δt, as it must be.

The Hamiltonian is symmetric under the simultaneous relabeling of atoms and sign change of δt: $[a, n \to b, n]$, $[b, n \to a, n+1]$, $[\delta t \to -\delta t]$. This transform is just moving the choosen unit cell over one atom. But the system doesn't know which atom we call a or b, so the system must also be symmetric under $[\delta t \to -\delta t]$. So the bandstructure can't change.

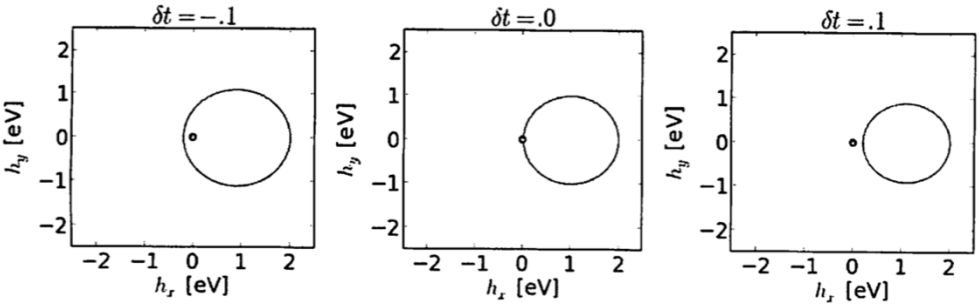
The representation of the states, however, does depend on our choice of unit cell placement (ie whether the strong coupling is intra-cell or inter-cell). So the eigenvectors can and do change under $\delta t \to -\delta t$. At the gap extremum ($k = \pm\pi/a$), we have $h_y = 0$, $h_x = 2\delta t$. So it's easy to see that the sign of h_x at the gap flips as one goes through $\delta t = 0$. This can be viewed more geometrically, as I'll show in the next part.

d)

From the explicit formula in (b), we see that $\vec{h}(k) = (h_x(k), h_y(k), 0)$ traces out a cirle in the $x-y$ plane of radius $t - \delta t$ centered on $t + \delta t$ as k goes from 0 to $\pm\pi/a$. So the sign of δt determines whether that circle reaches to the origin. For positive δt, the radius is smaller than the offset, so the circle is too small to touch the origin. For negative δt, the radius is larger than the offset, so the circle winds the origin.

```
def plotCirc(t,dt):
    k=linspace(-pi,pi)
    hx=(t+dt)+(t-dt)*cos(k)
    hy=(t-dt)*sin(k)
    plot(hx,hy)
    plot(0,0,'o')
    xlim(-2.5,2.5)
    ylim(-2.5,2.5)
    xlabel('$h_x$ [eV]')
    ylabel('$h_y$ [eV]')

figure(figsize=(11,4))
subplot(131)
plotCirc(1,-.1)
title('$\delta t=-.1$')
subplot(132)
plotCirc(1,0)
title('$\delta t=.0$')
subplot(133)
plotCirc(1,.1)
title('$\delta t=.1$')
tight_layout()
```



d)

(Yes, this is the second Problem 5.2(d) on this pset. What of it?)

The ϕ component of Berry connection (of the upper band) is

$$\mathcal{A}_\phi = i\langle +|\partial_k|+\rangle = i(\partial_k \phi)\langle +|\partial_\phi|+\rangle$$

Plugging in the eigenstates from the gauge chosen in (a), specifically where $\theta = 0$

$$\mathcal{A}_\phi = i(\partial_k \phi)\begin{pmatrix} e^{i\phi}\frac{1}{2} & \frac{1}{2}\end{pmatrix}\partial_\phi \begin{pmatrix} e^{-i\phi}\frac{1}{2} \\ \frac{1}{2}\end{pmatrix} = i(\partial_k\phi)\times(-i/2) = \frac{1}{2}\partial_k\phi$$

If we integrate over k from $-\pi/a$ to π/a, we get the Berry phase:

$$\gamma = \frac{1}{2}\int_{-\pi/a}^{\pi/a} dk\cdot\partial_k\phi$$

This integral can be determined by looking at the pretty pictures from the first Problem 5.2(d). There we see that, if $\delta t > 0$, then $\vec{h}$ doesn't enclose the origin, so $|\phi|$ can never go beyond $\pi/2$, thus ϕ can never complete a phase loop. It starts at zero, increases, and then decreases back to it's original value. Thus, $\int_{-\pi/a}^{\pi/a} dk\cdot\partial_k\phi = 0$. On the other hand, if $\delta t < 0$, then $\vec{h}$ encircles the origin once, so ϕ, monotonically increasing, completes a full cycle from 0 to $2\pi \equiv 0$, and $\int_{-\pi/a}^{\pi/a} dk\cdot\partial_k\phi = 2\pi$.

Hence, for $\delta t > 0$, $\gamma = 0$, and for $\delta t < 0$, $\gamma = \pi$.

This is like the Dirac monopole problem in that only paths which circle the z-axis (or whatever axis is picked out by your gauge choice) pick up a non-zero phase.

e)

In order to transform the bandstructure for a $\delta t < 0$ to a $\delta t > 0$ situation, as one must do when crossing the domain wall in this molecule, the loops of 5.2(d) must go from enclosing the origin to excluding the origin. Since the loops (however they may distort) must stay closed (by the periodicity of bandstructures), there must be some intermediate point where the loop includes the origin (as in the $\delta t = 0$ image). At such a point, $\vec{h}(\pi/a) = 0$, so the $k = \pm\pi/a$ states have zero energy, and the bands touch.

Problem 5.6: Survey of Topological Aspects of Quantum Transport

Problem 5.6) Survey of Topological Aspects of Quantum Transport

In class, I mentioned the 'zoo' of Hall-effects: the ordinary Hall effect → Integer Quantum Hall effect, the spin-Hall effect → the Quantum Spin-Hall Effect, the Anomalous Hall effect → the Quantum Anomalous Hall effect. Early in this class we also encountered quantization of conductance in ordinary 1D ballistic transport. Write a short summary in the form of a table of these effects, and what sorts of materials, temperatures, and fields (magnetic, electric) are required to observe these transport phenomena. In this table, also indicate the degree of robustness to disorder, and which of these are considered to be 'topologically protected'.

Solution: [By Andrei Isichenko, 2017]

Problem 6 — Survey of Topological Aspects of Quantum Transport.

Hall Effect	Summary	Materials	Temp	Fields	Robustness to disorder	Is "topologically protected"?
Ordinary Hall effect	Voltage difference transverse to an electric current and B field	semiconductors, conductors	room temp	E field, B field	Yes	No
Integer QHE	electrons in B field have quantized orbits (quantized energy) lead to magnetic flux quantization Definition	2DEG in materials like graphene, GaAs, ZnO-MgZnO	low, but up room temp sometimes	B field, small E field	need disorder, but not too much!	Yes, can be
Spin Hall Effect	spin accumulation on the lateral surfaces of an electric current-carrying sample. "spin current" caused by spin-orbit interaction.	semiconductors	room temp ?	only E field needed	N/A	No
Quant Spin Hall	also caused by S-O coupling in zero applied magnetic field.	special 2D semiconducting HgTe quantum wells graphene	< room temp	no large B field required	Yes	Yes
Anomalous HE	requires a combination of magnetic polarization and spin-orbit coupling to generate the Hall voltage in absence of B field	ferromagnetic conductors, e.g. Nickel	room temp	no B field	No	No
(4) Q.A.H.E.	quantized version of anom. HE. $\sigma = C\cdot e^2/h$, C is Chern #.	chern insulators	low temp	no field B	Yes	Yes