ECE 5390/MSE 5472, Fall Semester 2017
Quantum Transport in Electron Devices & Novel Materials

Debdeep Jena (djena@cornell.edu), Depts. of ECE and MSE, Cornell University

Assignment 5

Policy on assignments: Please turn them in by 5pm of the due date. The due date for this assignment is **Friday, Dec 8th, 2017**.

General notes: Present your solutions *neatly*. Do not turn in rough unreadable worksheets - learn to **take pride in your presentation**. Show the relevant steps, so that partial points can be awarded. $\boxed{\text{BOX}}$ your final answers. Draw figures wherever necessary. Please print out this question sheet and staple to the top of your homework. Write your name and email address on the cover. Some problems may lead to publishable results - be on the lookout!

Problem 5.1) The Berry Phase and Chern Numbers

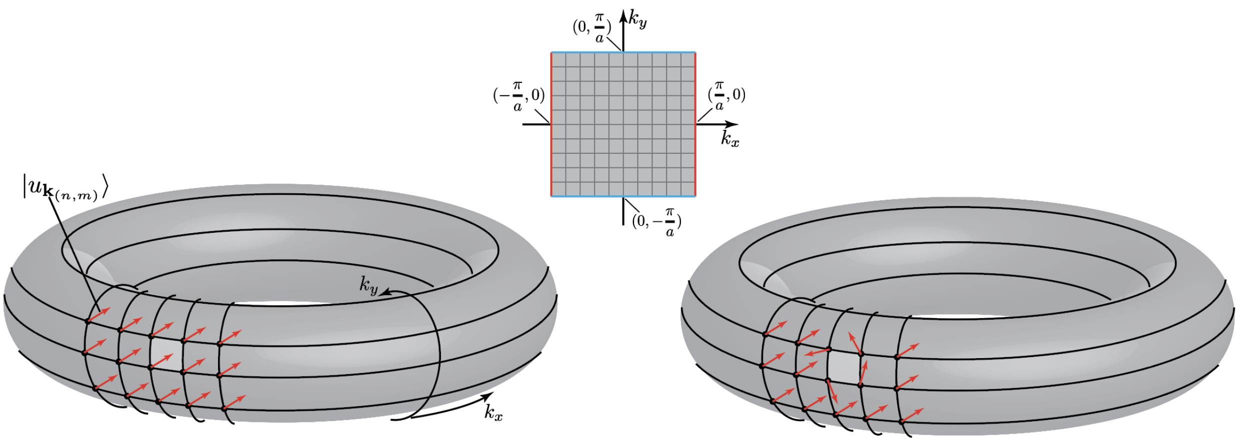

Figure 1: Berry phase and Chern Number.

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 $|\psi_{\mathbf{k}}\rangle \to e^{i\alpha_{\mathbf{k}}}|\psi_{\mathbf{k}}\rangle$, 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:

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

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

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

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

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

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.

Problem 5.2) Berry Phase and Berry Curvature

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:

[1] In the specific case of Bloch functions, the Berry phase is defined as $\gamma_L = i\oint d\mathbf{k} \cdot \langle u_{n\mathbf{k}} | \nabla_{\mathbf{k}} | u_{n\mathbf{k}} \rangle$, where $u_{n\mathbf{k}}$ is the cell-periodic part of the Bloch wavefunction. The modulating envelope function $e^{i\mathbf{k}\cdot\mathbf{r}}$ is pushed out to the Hamiltonian to make $\mathbf{k}$ the explicit parameter.

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 $\mathcal{K}'$?

Problem 5.3) Quantum Hall Effect and Chern Number

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

[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!

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

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

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.

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

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

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 $E_\pm = \frac{\hbar^2 k^2}{2m} \pm \sqrt{\lambda^2 k^2 + \Delta^2}$. 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 $-\Delta \leq E_F \leq \Delta$ and drops rapidly outside the window.

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

Problem 5.5) Topological Insulators, Winding Number, Berry Phase

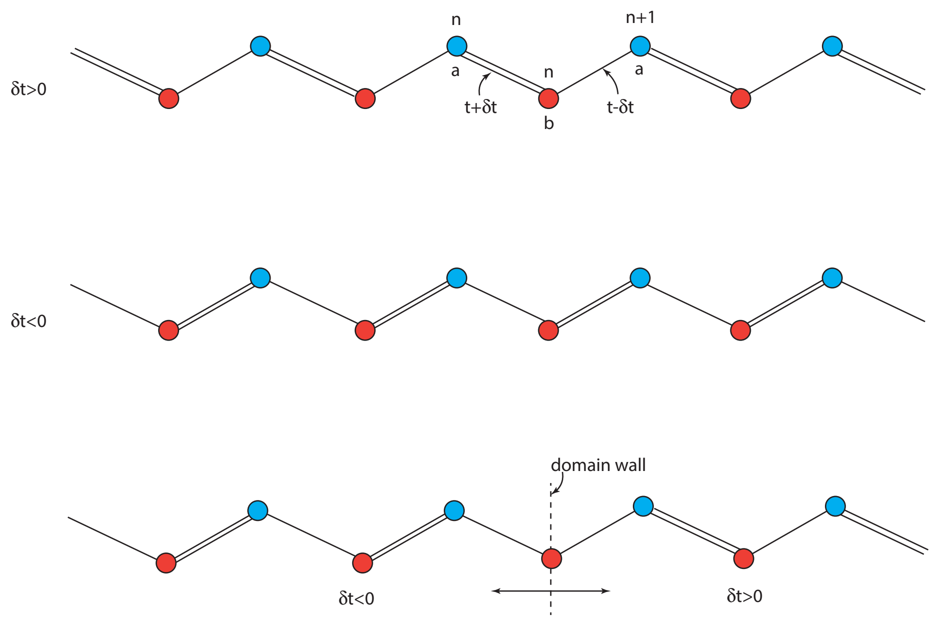

Figure 2: A polyacetylene chain that exhibits a non-trivial topological feature in its bandstructure.

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'.

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'.