Policy on assignments: Please turn them in by 5pm of the due date. The due date for this assignment (=Exam) is **Friday, Dec 11th, 2015**.

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. ⎡ 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) Berry Phase and the Quantum Hall Effect

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 $|\mathcal{K}\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{2}}\left(\begin{smallmatrix}1\\e^{-i\theta}\end{smallmatrix}\right)$ and $|\mathcal{K}'\rangle = \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{2}}\left(\begin{smallmatrix}1\\e^{+i\theta}\end{smallmatrix}\right)$, 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 $\Omega(\mathbf{k}) = \nabla \times \mathcal{A}(\mathbf{k})$ 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:

$$\Omega_{\mu\nu}(\mathbf{k}) = i[\langle\frac{\partial u_n}{\partial k_\mu}|\frac{\partial u_n}{\partial k_\nu}\rangle - \langle\frac{\partial u_n}{\partial k_\nu}|\frac{\partial u_n}{\partial k_\mu}\rangle] = i\sum_{n'\neq n}\frac{\langle n|\frac{\partial\hat{H}}{k_\mu}|n'\rangle\langle n'|\frac{\partial\hat{H}}{k_\nu}|n\rangle - \langle n|\frac{\partial\hat{H}}{k_\nu}|n'\rangle\langle n'|\frac{\partial\hat{H}}{k_\mu}|n\rangle}{(E_n - E_{n'})^2} \quad (1)$$

(c) We discussed that the traditional textbook formula for 'group velocity' of electronic states in

bands misses out the term due to the Berry curvature of the bandstructure. This factor has assumed increased importance since its association with the robustness of the quantum Hall effect. Assume Bloch-state electrons in a crystal with eigenstates of the nth band given by $\psi_{nq}(r) = e^{iqr}u_{nq}(r)$. Show that the modified formula for the expectation value of the group velocity of electrons in a band is

$$v_n(q) = \frac{1}{\hbar}\frac{\partial E_n(q)}{\partial q} - \Omega_{qt} \tag{2}$$

where $\Omega_{qt} = i[\langle\partial_q u_n|\partial_t u_n\rangle - \langle\partial_t u_n|\partial_q u_n\rangle]$ is the Berry curvature of the band in the (q,t) parameter space. The curvature term makes it possible for a *filled band* to contribute to electrical conductivity tensors. The integral of this Berry curvature over the entire Brillouin zone is called the Chern number, which is an integer - the same integer of the integer quantum Hall effect. Make a connection between the result of part (b) of this problem, with the quantized hall conductance.
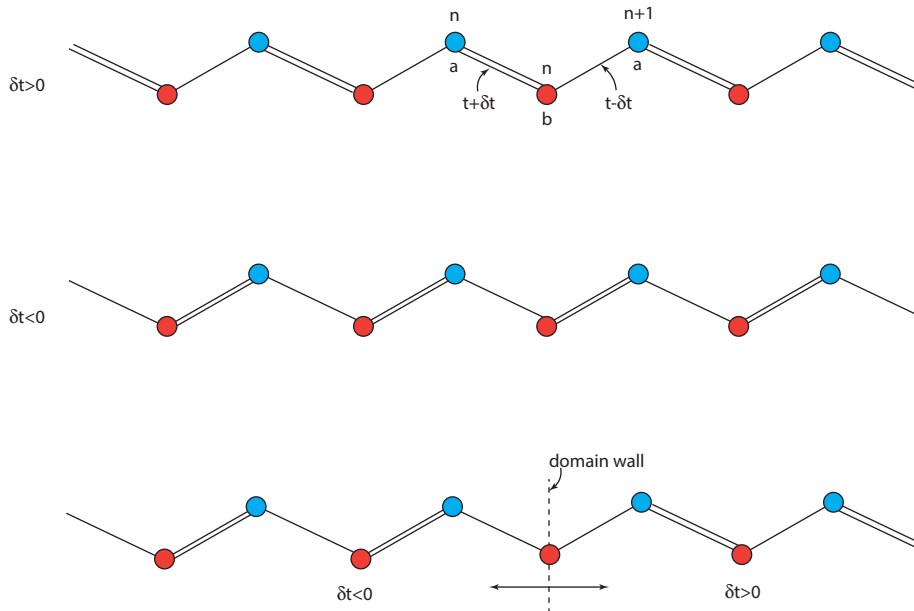
Problem 5.2) The SSH Model of a Topological Insulator

Figure 1: 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 $H_2 = \begin{pmatrix} h_0(k)+h_z(k) & h_x(k)-ih_y(k) \\ h_x(k)+ih_y(k) & h_0(k)-h_z(k) \end{pmatrix}$, and can be decomposed into the form $H_2 = h_0(k)I+h_x(k)\sigma_x+h_y(k)\sigma_y+h_z(k)\sigma_z = h_0(k)I + \vec{h}\cdot\vec{\sigma}$, 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 1) 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 $H = \sum_n \left(\left[(t + \delta t) c_{a,n}^\dagger c_{b,n} + (t - \delta t) c_{a,n+1}^\dagger c_{b,n} \right] + \left[c.c. \right] \right)$ in the occupation number formalism. Show that the resulting $k-$space Hamiltonian is $H = \int \frac{dk}{2\pi} \left(c_{a,k}^\dagger \ c_{b,k}^\dagger \right) \begin{pmatrix} h_0(k)+h_z(k) & h_x(k)-ih_y(k) \\ h_x(k)+ih_y(k) & h_0(k)-h_z(k) \end{pmatrix} \begin{pmatrix} c_{a,k} \\ c_{b,k} \end{pmatrix}$, 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 1), 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 5.3) Electron-Electron interactions in transport through a Q-Dot

Here you analytically and numerically show using the occupation-number picture why when electron transport occurs through a quantum dot that has *two* degenerate allowed energies, the conductance goes through a '2/3' step. This is the simplest manifestation of the *electron-electron interaction* effect in charge transport. Assume identical contact couplings $\gamma_1 = \gamma_2 = \gamma = 1$ eV, and the single-particle quantum-dot energies $E_0 = 2$ eV. Fix $\mu_2 = 0$ eV, and vary the potential of the left contact $\mu_1 - \mu_2 = qV$. Make plots of $I - V$ at 500K, 300K, and 10K for transport through the dot when the electron-electron interaction potential (the 'Hubbard' term) changes from $U = 0$ eV to $U = 1$ eV.

Problem 5.4) Second Quantization methods and quasiparticles

To handle interactions between many particles, we introduced the occupation-number (or Fock-space) formalism of quantum mechanics through the creation and annihilation operators that obeyed the relations $[b_i, b_j^\dagger] = b_i b_j^\dagger - b_j^\dagger b_i = \delta_{ij}$ for Bosons, and $\{c_i, c_j^\dagger\} = c_i c_j^\dagger + c_j^\dagger c_i = \delta_{ij}$ for Fermions. The creation and annihilation operators follow the ladder operations $b^\dagger |n\rangle = \sqrt{n+1}|n+1\rangle$ and $b|n\rangle = \sqrt{n}|n-1\rangle$ for bosons, and corresponding relations for Fermions. The Pauli-exclusion principle is built into this formalism from the get-go because the occupation number of an orbital for Fermions can be only 0, or 1, the only possible eigenvalues of the occupation number operator $\hat{N} = c^\dagger c$.

For Bosons, we could create a Fock-state $|\Psi\rangle = |n_1, n_2, ..., n_k, ...\rangle$ by repeated application of the creation operator on the Vacuum state: $|\Psi\rangle = |n_1, n_2, ..., n_k, ...\rangle = \frac{(b_k^\dagger)^{n_k}}{\sqrt{n_k!}} ... \frac{(b_2^\dagger)^{n_2}}{\sqrt{n_2!}} \frac{(b_1^\dagger)^{n_1}}{\sqrt{n_1!}}|0\rangle$. Since the Bosonic creation and annihilation operators of different orbitals *commute*, we do not have to worry about the *order* in which the creation operators act on the vacuum state. The vacuum state $|0\rangle = |0, 0, 0, ...\rangle$ has all orbitals unoccupied, and formally looks the same for Bosons and Fermions. Similarly, we could create a Fermionic Fock state by repeated application of the creation operators on $|0\rangle$, but since the creation operators of different orbitals *anti-commute*, we have to pay special attention to the ordering: $|\Psi\rangle = |n_1, n_2, ..., n_k, ...\rangle = (c_k^\dagger)^{n_k} ... (c_2^\dagger)^{n_2}(c_1^\dagger)^{n_1}|0\rangle$. Note that since $n_j = 0$ or 1 for Fermions, $\sqrt{n_j!} = 1$ for all, so we do not need to write out the factorials.

(a) Show that the fermion anti-commutator algebra directly implies $(\hat{c}_\lambda^\dagger)^2 = 0$. Argue why this is nothing but the Pauli exclusion principle for fermions, meaning $\hat{n}_\lambda = \hat{c}_\lambda^\dagger \hat{c}_\lambda$ acting on fermion eigenstates can only produce eigenvalues 0 or 1, unlike $0, 1, 2, ...$ for bosons.

Evaluate the following matrix elements (Note that $a = b$ and $a^\dagger = b^\dagger$ for bosons, and $a = c$ and $a^\dagger = c^\dagger$ for Fermions, a is simply a more general creation/annihilation operator symbol):

(b) $\langle 1, 1|a_1^\dagger a_2^\dagger a_1 a_2|1, 1\rangle$ for Bosons ($a = b$), and then Fermions ($a = c$), and compare the results with $\langle 1, 1|a_1^\dagger a_1 a_2^\dagger a_2|1, 1\rangle$.

(c) $\sum_{j=1}^{\infty}\langle ...0_{k+1}, 1_k, ..., 1_2, 0_1|a_j^\dagger a_j|0_1, 1_2, ..., 1_k, 0_{k+1}, ...\rangle$ for Fermions and then for Bosons.

The ground state of an electron (Fermion) system may be written as $|\Phi\rangle = |1_1, 1_2, ..., 1_N, 0_{N+1}, ...\rangle$, where N is the highest occupied orbital (its energy E_N is the Fermi energy). Work out the following matrix element sums for $|\Phi\rangle$:

(d) $\sum_{j,k,l,m}^{\infty}\langle \Phi|a_j^\dagger a_k^\dagger a_l a_m|\Phi\rangle = 0$.

(e) $\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N}\sum_{m=1}^{N}\langle \Phi|e^{i(l-k)x}a_j^\dagger a_k^\dagger a_l a_m|\Phi\rangle = N^2 - \frac{\sin^2(\frac{Nx}{2})}{\sin^2(\frac{x}{2})} = G_N(x)$. Make a sketch of the function $\frac{G_N(x)}{N^2}$ as a function of x for various (large) values of N. This function is called the pair-correlation function.

Solve the following simple yet profound problem. In the Bardeen-Cooper-Schrieffer (BCS) theory of superconductivity, the annihilation and creation operators for a correlated pair of electrons of opposite spins (the Cooper-pair) are defined by $\hat{a}_{\mathbf{k}} = \hat{c}_{-\mathbf{k},\downarrow}\hat{c}_{\mathbf{k},\uparrow}$ and $\hat{a}_{\mathbf{k}}^\dagger = \hat{c}_{\mathbf{k},\uparrow}^\dagger \hat{c}_{-\mathbf{k},\downarrow}^\dagger$.

(f) Show that $[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k'}}] = [\hat{a}_{\mathbf{k}}^\dagger, \hat{a}_{\mathbf{k'}}^\dagger] = 0$.
(g) Show that $[\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k'}}^\dagger] = \delta_{\mathbf{k},\mathbf{k'}}(1 - \hat{n}_{-\mathbf{k},\downarrow} - \hat{n}_{\mathbf{k},\uparrow})$.
(h) Show that $\{\hat{a}_{\mathbf{k}}, \hat{a}_{\mathbf{k'}}\} = 2\hat{a}_{\mathbf{k}}\hat{a}_{\mathbf{k'}}(1 - \delta_{\mathbf{k},\mathbf{k'}})$.

(i) Argue from the above algebra that Cooper pairs *seem* to follow boson algebra for 'hole' states, when $\hat{n}_{-\mathbf{k},\downarrow} = \hat{n}_{\mathbf{k},\uparrow} = 0$, *even though they are made of fermions!*. But also argue why their creation/annihilation algebra is not *exactly* bosonic.

(j) Discuss how particles of different types (fermions & bosons) may be treated by the 2nd quan-

tization techniques. Identify the importance of diagonalization of the many-particle Hamiltonians, and how this process predicts quasiparticles such as excitons, polarons, or polaritons - all of which have been experimentally observed.

Problem 5.5) Cooper pairs in Superconductors

In this problem, we expose the limitations of perturbation theory in quantum mechanics. The reason why it took nearly half a century from the experimental discovery of superconductivity to the development of a theory for it is because its physics cannot be obtained from perturbation theory. One has to solve the Hamiltonian problem more or less *exactly* - even if for a simplified toy model that captures the essential physics. Now Bardeen, Cooper, and Schrieffer (BCS) constructed such a theory. We first solve the toy model that Cooper did to unlock the mystery.

(a) Working in the Fourier (k-)space, show that for an electron of mass m moving in 1D with an attractive Dirac-delta potential $V(x) = -\alpha\delta(x)$, there is *exactly* one bound state, no matter how small the strength α. Show that this bound-state energy is $E_0 = -\frac{m\alpha^2}{2\hbar^2}$.

(b) Following (a), set up the same problem for a $D-$dimensional Dirac-delta attractive potential for an electron moving in $D-$dimensions. Show why a naive search for bound states leads to divergent $k-$space integrals for $D > 1$. Fact: theorists just *love* such divergences!

(c) Tame the *ultraviolet divergence* as $k \to \infty$ by imposing an *ultraviolet cutoff* of $k_{max} = \frac{1}{a}$. This is a fancy way of saying that we will set a minimum floor on the wavelengths permitted for electrons. Find the required condition for bound states in $D-$dimensions with this UV cutoff.

(d) Now a great many profound physics discoveries have resulted from studying the long-wavelength, or the *infrared divergences*. This happens when integrals blow up as $k \to 0$, or electron wavelengths become very long. Show that for a *vanishingly weak* Delta-function $\alpha \to 0$, there cannot be a bound state for $D \geq 3$.

(e) Show that for $D = 2$, there is a bound state of energy $E_0 = -\frac{\hbar^2}{ma^2(e^{\frac{2\pi\hbar^2}{m\alpha}}-1)} \approx -\frac{\hbar^2}{ma^2}e^{-\frac{2\pi\hbar^2}{m\alpha}}$ for a vanishingly small attractive Dirac-delta potential as $\alpha \to 0$. Explain why this result is unattainable from perturbation theory.

(f) Now make the connection of the toy problem to the Cooper pair problem: two electrons of opposite spins at the Fermi energy surface $E_F = \frac{p_F^2}{2m}$ of a metal bound by a phonon of energy $\hbar\omega_0$ via a vanishingly weak potential $V(r) = -V_0\delta(r)$. Since the Fermi-surface is 2D, show that one obtains an effective superconductive gap $\Delta = -(\hbar\omega_0)e^{-\frac{1}{N_0 V_0}}$, where $N_0 = \frac{mp_F}{4\pi^2\hbar^3}$. Discuss why the gap is small, and why it cannot be obtained from perturbation theory.