Departments of ECE and MSE, Cornell University

ECE 4070/MSE 5470: Physics of Semiconductor and Nanostructures

Spring 2015

Homework 8 **Due on May 1, 2015 at 5:00 PM**

Suggested Readings:

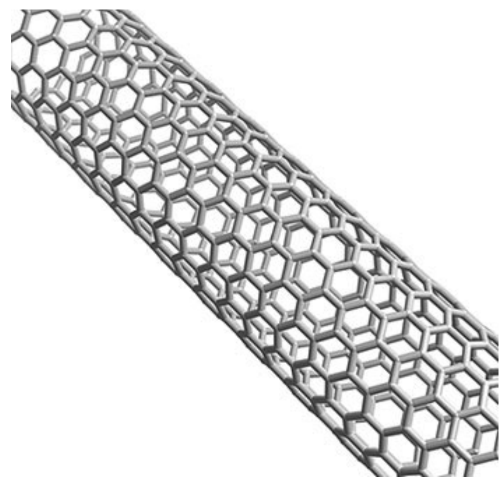
a) Lecture notes

Problem 8.1 (ZigZag Carbon Nanotubes)

The energy band dispersion of graphene can be written as,

$$E(\vec{k}) = E_p \pm \hbar v \sqrt{(k_x - K_{xp})^2 + (k_y - K_{yp})^2}$$

where (K_{xp}, K_{xp}) is the location of the vertex of the Brillouin zone (the "*K*" point). The gap at this point is zero for 2D graphene – as you have done before.



Consider a semiconducting zizag nanotube made by "rolling up" graphene with circumference given by $C = ma_0$ where a_0 is the lattice constant, and m an integer that is not a multiple of 3. Also $C = 2\pi R$ where R is the radius of the nanotube. Assume that $C >> a_0$.

a) Show that the bandgap is $E_g = {2\hbar v}/{3R}$. What is the magnitude (in eV) of the bandgap for a 1 nm radius zigzag nanotube?

b) The total electron density $\boldsymbol{n}$ (units: #/m) at the bottom of the two lowest (and degenerate) conduction bands can be written as:

$$\boldsymbol{n = \int_{E_p + \frac{E_g}{2}}^{\infty} g_{1D}(E)\, f(E - E_f)\, dE}$$

Find the conduction band density of states function $\boldsymbol{g_{1D}(E)}$ for the nanotube and sketch it. Don't forget to include band as well as spin degeneracies in $\boldsymbol{g_{1D}(E)}$.

c) Suppose T=0K. Find an expression relating the electron density $\boldsymbol{n}$ to the Fermi energy $\boldsymbol{E_F}$ by evaluating the integral in part (b) exactly.

d) Sometimes it is helpful to assign effective masses to the carriers near the band edges in semiconducting nanotubes even though the energy band dispersion is not exactly parabolic. Show that the 1D energy subband dispersions for the conduction and valence bands of a semiconducting zigzag nanotube of radius $\boldsymbol{R}$ can be **approximately** written right near the band edges in the following parabolic forms:

$$E_c(k_x) \approx E_p + \frac{E_g}{2} + \frac{\hbar^2 k_x^2}{2m_e} \qquad E_v(k_x) \approx E_p - \frac{E_g}{2} - \frac{\hbar^2 k_x^2}{2m_h}$$

and find expressions for the electron and hole effective masses m_e and m_h. Would the electrons and holes be lighter or heavier in nanotubes of larger radii?

Problem 8.2 (Ballistic Transistor Characteristics and Quantum Effects)

In class, we derived the characteristics of a ballistic field-effect transistor. You are going to fill in a few steps, and solve a closely related problem.

a) Make (log-scale and linear-scale) plots of the gate-induced 2D electron gas (2DEG) carrier density at 300K and 77K vs the gate voltage of FETs for an insulating barrier of $t_b = 2$ nm, $\varepsilon_b = 10\varepsilon_0$ for three semiconductor channels: one that has $m_c^* = 0.2m_0$, $g_s = 2$, $g_v = 2$, the second has $m_c^* = 0.2m_0$, $g_s = 2$, $g_v = 1$, and the third has $m_c^* = 0.05m_0$, $g_s = 2$, $g_v = 1$. What is the difference? [see Fig 10.2 of notes for a representative figure]
b) Show why the ballistic current density is given by $J_{2d} = J_0[F_{1/2}(\eta_s) - F_{1/2}(\eta_s - v_d)]$, where $J_0 = q\sqrt{4\pi}\frac{\hbar N_c}{m_c^*}$, and all symbols have their usual meanings (as they appear in the notes/handouts, N_c is the effective conduction band edge DOS).
c) Make a plot of the ballistic FETs of the three semiconductors of part (a). Make the drain current vs gate voltage and drain current vs drain voltage plots, similar to Fig 10.4.
d) Describe qualitatively what sorts of changes in the device characteristics would you expect if instead of the 2DEG channel, you had a 1D channel in the ballistic FET. Specifically, show that the ballistic conductance per 1D channel is limited to the quantum of conductance, where $G_0 = g_s g_v \frac{q^2}{h}$ where h is the Planck's constant.

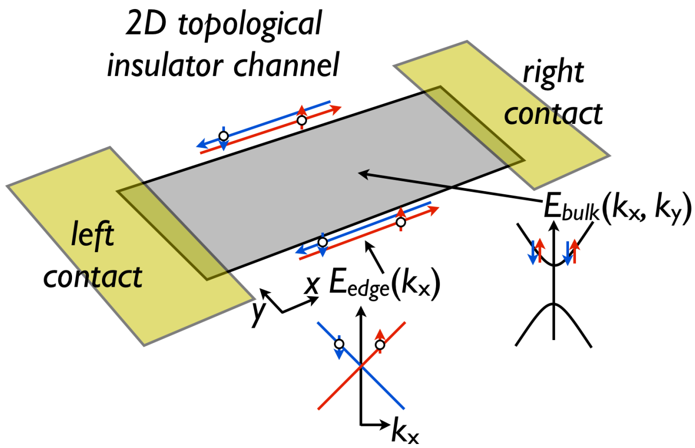
Problem 8.3 (Topological Insulator Field-Effect Transistors)

A topological insulator is a crystal that has a strong coupling of the spin to the crystal momentum of the electron resulting in a strange feature in the energy bandstructure. The upshot of the effect of geometry and topology on the electron Bloch functions is this: there are certain crystals for which the energy bandstructure $E_{bulk}(k_x, k_y)$ of the bulk ("interior") of the crystal is similar to a traditional semiconductor and has a bandgap. But there are zero-gap bands $E_{surf}(k_x)$ attached to the surface (or edge) that are topological in origin. Just like one can smoothly deform a donut into a coffee cup (both have one hole), but one cannot deform a donut into a sphere, it turns out that the surface (or edge) states are robust and one cannot get rid of them in these materials, called Topological Insulators.

In this problem, we consider a 2D Topological Insulator (TI) material as the channel of a ballistic FET, and borrow heavily from the results of Problem 8.2 above to gain insight to transport in them.

a) You have solved the ballistic FET problem with a 2DEG channel of width W. Sketch a $\log(I_d) - V_{gs}$ curve of a ballistic FET that is a normal semiconductor with a gapped bulk bandstructure $E_{bulk}(k_x, k_y)$, and that has NO topological edge states.
b) Now consider that this channel is indeed a TI, and has additional one-dimensional topological edge states $E_{surf}(k_x)$ along the physical edges of the 2DEG, separated in space by W. Because of the spin-momentum locking, in these edge states the right-going and left-going states have

opposite spins (this is a *key* idea of a TI!). In other words, the spin-degeneracy of the right-going state is not 2, but 1 – and all right-going carriers have the same (say, up) spin, which is opposite to the spin (down) of all the left going carriers. This is shown schematically in the figure below. Consider the dispersion of the edge states to be $E_{surf}(k_x) = \hbar v_F k_x$, and show that the ballistic conductance of *each* edge channel is $G_0 = \frac{q^2}{h}$, even after taking the spin into account. Compare with your answer in Problem 8.2 (d).



c) From the figure above, show that the net ballistic conductance of the two topological edge channels is $G_0 = 2\frac{q^2}{h}$, no matter what the gate voltage.

d) Sketch how this modifies the $\log(I_d) - V_{gs}$ curve that you sketched in part (a). What is the minimum conductance?

e) Explain why this sort of behavior cannot be obtained if I took a Silicon MOSFET and attached two conventional semiconducting 1D quantum wires at the two edges. What would the conductance minimum be then? If you have got to this point, you should be able to understand this paper that lays claim to be the first experimental observation of a TI state: Science vol 318, pg 766-770, 2007. Especially look at Fig 4 and compare with your sketch in (d).

f) If you can find an alternate explanation of the results observed in the paper, you can publish your results – this is a matter that is far from resolved!

Problem 8.4 (Boltzmann Transport in d-dimensions)

We derived the solution to the Boltzmann transport equation in the relaxation-time approximation for elastic scattering events to be $f(\mathbf{k}) \approx f_0(\mathbf{k}) + \tau(\mathbf{k})(-\frac{\partial f_0(\mathbf{k})}{\partial \varepsilon(\mathbf{k})})\mathbf{v_k} \cdot \mathbf{F}$, where all symbols have their usual meanings. Use this to show that for transport in d dimensions in response to a constant electric field E, in a semiconductor with an isotropic effective mass m^*, the current density is given by $J = \frac{nq^2\langle\tau\rangle}{m^*}E$, with $\langle\tau\rangle = \frac{2}{d} \cdot \frac{\int d\varepsilon \cdot \tau(\varepsilon)\varepsilon^{\frac{d}{2}}(-\frac{\partial f_0(\varepsilon)}{\partial \varepsilon})}{\int d\varepsilon \cdot \varepsilon^{\frac{d}{2}-1} f_0(\varepsilon)}$, where the integration variable $\varepsilon = \varepsilon(\mathbf{k})$ is the kinetic energy of carriers.

You have now at your disposal the *most general* form of conductivity and mobility from the Boltzmann equation for semiconductors that have a parabolic bandstructure!

Hints: The volume of a d-dimensional sphere in **k**-space is $V_d = \frac{\pi^{\frac{d}{2}} k^d}{\Gamma(\frac{d}{2}+1)}$, and the corresponding surface area is $S_d = \nabla_k V_d = \frac{d\pi^{\frac{d}{2}} k^{d-1}}{\Gamma(\frac{d}{2}+1)}$. Here $\Gamma(...)$ is the Gamma function with the properties $\Gamma(x+1) = x \cdot \Gamma(x)$ and $\Gamma(\frac{1}{2}) = \sqrt{\pi}$. Verify that these formulae give you the familiar 'volume' and 'surface area' for d=3 (sphere) and d=2 (circle). You may (or may not, depending on your approach) need the DOS of parabolic bands in d dimensions: $g_d(\varepsilon) = \frac{g_s g_v}{2^{d-2}\pi^{\frac{d}{2}}\Gamma(\frac{d}{2})}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{d}{2}} \varepsilon^{\frac{d}{2}-1}$. Again, plug in d=3, 2, and 1, and you should recover familiar expressions for DOS in different dimensions.

Problem 8.5 (Scattering from uncorrelated events)

Show using Fermi's golden rule that if the scattering rate of electrons in a band of a semiconductor due to the presence of ONE scatterer of potential $W(\mathbf{r})$ centered at the origin is $S(\mathbf{k} \to \mathbf{k}') = \frac{2\pi}{\hbar} |\langle \mathbf{k}' | W(\mathbf{r}) | \mathbf{k} \rangle|^2 \delta(E_{\mathbf{k}} - E_{\mathbf{k}'})$, then the scattering rate due to N_s scatterers distributed randomly and uncorrelated in 3D space is $N_s \cdot S(\mathbf{k} \to \mathbf{k}')$. This argument is subtle, and effects of interference should enter your analysis.

Hints: Add the potentials of each randomly distributed impurity for the total potential $W_{tot}(\mathbf{r}) = \sum_i W(\mathbf{r} - \mathbf{R}_i)$. Use the effective mass equation for the electron states to show that the matrix element is a Fourier transform. Then invoke the shifting property of Fourier transforms.