ECE 5390/MSE 5472, Fall Semester 2017

# Quantum Transport in Electron Devices & Novel Materials

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## Assignment 4

**Policy on assignments**: Please turn them in by 5pm of the due date. The due date for this assignment is **Monday, Nov 20th, 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 4.1) Survey of Superconductivity

Create a well-thought out table of the experimental status of various superconducting materials and their transport and related properties such as critical parameters $T_c$, $H_c$, $J_c$, gaps $\Delta$, London penetration depths $\lambda_L$, material stability, and other parameters you consider important. Include high-$T_c$ superconductors, and superconductors that are semiconductors under normal conditions. Indicate in the table which ones are used for industrial applications, and for what.

## Problem 4.2) Current Transport in Josephson Junctions

We have discussed how the Ginzburg-Landau theory explains superconductivity by introducing the macroscopic wavefunction $\Psi(r) = \sqrt{n(r)}e^{i\theta(r)}$, and in one masterstroke explains all the hallmarks of transport and related properties of superconductors such as persistent currents, the Meissner effect and London penetration depths, flux quantization, etc. This theory is also central to understanding most superconducting quantum devices, the Josephson junction being a prime example.
In class I outlined how to understand the rather remarkable current-voltage characteristics of a superconductor/insulator/superconductor junction in which Cooper pairs can tunnel from one superconductor to the other, leading to the flow of a ac Josephson current

$$I = I_0 \sin(\frac{2eV}{\hbar}t + \alpha), \tag{1}$$

where all terms have their usual meanings. Using the Landau-Ginzburg macroscopic wavefunctions $\Psi_1 = \sqrt{n_1}e^{i\theta_1}$ and $\Psi_2 = \sqrt{n_2}e^{i\theta_2}$ and using Schrodinger equation allowing for tunneling from one superconductor to the other, show that the current given by Equation 1. Assume $n_1 \approx n_2$. Discuss what is rather remarkable about the transport in this superconducting device, and show that $V \approx 1$ mV across the tunnel diode leads to an oscillation frequency of $\sim 3$ THz. Explain how such junctions are used in SQUID magnetometers.

## Problem 4.3) 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 $\alpha$. 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 this toy problem to the Cooper pair[1] problem we have discussed in class: two electrons of opposite momenta and opposite spins at the Fermi energy surface $E_F$ of a metal bound by phonons of energy up to $\hbar\omega_D$ via a vanishingly weak pairing potential $-V_0$. Show how the pairing causes the 2-electron energy to reduce from $2E_F \to 2E_F - \Delta$, where $\Delta = (2\hbar\omega_D)e^{-\frac{2}{N_0 V_0}}$, where $N_0$ is the DOS at the Fermi energy. Discuss why the gap is small, and why it cannot be obtained from perturbation theory.

## Problem 4.4) The BCS Theory of Superconductivity

**(a)** Show that an estimate of the critical current density that converts a superconductor of gap $\Delta$ to a normal metal is $J_c \approx 2en\frac{\Delta}{\hbar k_F}$, where $n$ is the normal single-particle electron density, $e$ the electron charge, and $k_F$ is the Fermi wavevector. Show that for standard metals it evaluates to $J_c \sim 10^7$ A/cm$^2$. (You can imagine that the superconducting gap prevents scattering, till the single particle states have kinetic energies larger than the gap. Another way to picture this is to estimate the electron kinetic energy needed to break the Cooper pairs.)

In class we discussed the BCS Hamiltonian is

$$H_{BCS} = \sum_{\mathbf{k},\sigma} E_0(\mathbf{k}) c^\dagger_{\mathbf{k}\sigma} c_{\mathbf{k}\sigma} - V_0 \sum_{\mathbf{k},\mathbf{q}} c^\dagger_{\mathbf{q}\uparrow} c^\dagger_{-\mathbf{q}\downarrow} c_{-\mathbf{k}\downarrow} c_{\mathbf{k},\uparrow}, \tag{2}$$

[1] Cooper, Leon N. (1956). "Bound electron pairs in a degenerate Fermi gas". Physical Review. 104 (4): 1189.

and the BCS macroscopic wavefunction is

$$|\Psi_{BCS}\rangle = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow})|0\rangle = \prod_{\mathbf{k}}(u_{\mathbf{k}} + v_{\mathbf{k}} b^{\dagger}_{\mathbf{k}})|0\rangle, \tag{3}$$

where $b^{\dagger}_{\mathbf{k}} = c^{\dagger}_{\mathbf{k}\uparrow} c^{\dagger}_{-\mathbf{k}\downarrow}$ is the Cooper pair creation operator with the corresponding annihilation operator $b_{\mathbf{k}} = c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow}$. In Problem 2.2, you have seen that these operators composed of two fermionic operators look somewhat like Boson operators, but are not quite Bosonic. The terms $u_{\mathbf{k}}$ and $v_{\mathbf{k}}$ are unknown coefficients. For our purposes, assume them to be real (though this is not necessary).

**(b)** Show how normalization of the BCS macroscopic wavefunction $\langle\Psi_{BCS}|\Psi_{BCS}\rangle = 1$ followed by the minimization of the energy $\langle\Psi_{BCS}|H_{BCS}|\Psi_{BCS}\rangle$ gives us the $T << T_c$ K Cooper pair occupation function

$$v^2_{\mathbf{k}} = \frac{1}{2}[1 - \frac{E_0(\mathbf{k}) - E_F}{\sqrt{(E_0(\mathbf{k}) - E_F)^2 + \Delta^2}}], \tag{4}$$

where $\Delta$ is the *superconducting gap* given by $\Delta = -V_0 \sum_{\mathbf{k}} u_{\mathbf{k}} v_{\mathbf{k}}$. Make a plot of this function, and compare it with the single-particle non-interacting Fermi-Dirac function choosing appropriate numerical values.

**(c)** Using the earlier part on occupation functions, show that the *condensation energy*, or energy reduction for electrons to make a transition from the normal metallic to the superconducting state is $\mathcal{U}_{sc} - \mathcal{U}_m = -\frac{1}{2} N_0 \Delta^2$.

**(d)** I outlined in class how to obtain excited state properties from the BCS theory using the Bogoliubov de-Gennes approach instead of the variational approach. Show how this approach diagonalizes the BCS Hamiltonian in Equation 2 to the form

$$H_{BdG} = \sum_{\mathbf{k}} E_{BdG}(\mathbf{k})(\gamma^{\dagger}_{\mathbf{k}\uparrow}\gamma_{\mathbf{k}\uparrow} + \gamma^{\dagger}_{-\mathbf{k}\downarrow}\gamma^{\dagger}_{-\mathbf{k}\downarrow}), \tag{5}$$

where the quasiparticles have an energy spectrum $E_{BdG}(\mathbf{k}) = \sqrt{(E_0(\mathbf{k}) - E_F)^2 + \Delta^2}$. Write the relation between the creation/annihilation operators $\gamma_{\mathbf{k}}$'s and the original $c_{\mathbf{k}}$'s. Write the commutation relations of these new operators and comment.

**(e)** Outline how the temperature-dependent properties of the superconductor, say the gap $\Delta(T)$ may be obtained from the BCS type theory.