P502	Problem set # 5	Due: Dec. 6, 14:30

1. (25 points) *"Thermally activated conductivity in a band insulator"* When the Fermi level lies inside the band gap all the energy bands in the solid are either filled or empty and, as a result, electrical conductivity vanishes. However, this statement is strictly true only at $T = 0$. At any nonzero temperature electrons will be thermally excited across the gap giving rise to a finite population of electrons in the upper (conduction) band and holes in the lower (valence) band. These thermally activated carriers then produce nonzero conductivity in the insulator. In this problem we examine a simple generic model for such thermally activated conductivity.

Consider a *two dimensional (2D)* system whose energy spectrum in the vicinity of the Fermi level is described by

$$\epsilon(\mathbf{k}) = \pm\left(\Delta + \frac{\hbar^2\mathbf{k}^2}{2m^*}\right). \tag{1}$$

Here $\mathbf{k}^2 = k_x^2 + k_y^2$ (we are in 2D), $2\Delta > 0$ is the band gap and Fermi energy is $\epsilon_F = 0$. The dispersion (1) can be thought of as a generic expansion of the energy near the isotropic band maximum/minimum and is frequently used in semiconductor physics.

a) Calculate the density of states $\rho(\epsilon)$. Sketch $\rho(\epsilon)$ and indicate which levels are filled/empty at $T = 0$ and $T > 0$. Show that chemical potential will remain pinned at zero energy even at $T > 0$.

b) As a warm-up exercise calculate the specific heat $c_v(T)$ and show that it can be written as

$$c_v(T) = \mathcal{C}_1 \int_\Delta^\infty d\epsilon \frac{(\beta\epsilon)^2}{\cosh^2(\frac{1}{2}\beta\epsilon)} \tag{2}$$

where $\beta = 1/k_BT$ and $\mathcal{C}_1$ is a T-independent prefactor. Determine $\mathcal{C}_1$.

c) Find the leading T-dependence of $c_v(T)$ in the limiting cases $k_BT \ll \Delta$ and $k_BT \gg \Delta$. Show that in the former case specific heat becomes exponentially activated, $c_v(T) \sim e^{-\Delta/k_BT}$. What is the behavior in the opposite limit, $k_BT \gg \Delta$? Give the physical interpretation of these limiting forms.

d) Derive the exact result for DC electrical conductivity within the relaxation time approximation assuming constant τ. Show that it can be written in the form

$$\sigma_{\mu\nu} = \mathcal{C}_2 \delta_{\mu\nu} \int_\Delta^\infty d\epsilon \frac{\beta(\epsilon - \Delta)}{\cosh^2(\frac{1}{2}\beta\epsilon)} \tag{3}$$

where $\beta = 1/k_BT$. Determine $\mathcal{C}_2$. Examine the properties of the integral in Eq. (3) and find the leading T-dependence of $\sigma_{\mu\nu}$ in the limiting cases of $k_BT \ll \Delta$ and $k_BT \gg \Delta$.

e) Neglecting the electro-thermal effects calculate the thermal conductivity $\kappa_{\mu\nu}$ within the same set of approximations as above. Is Wiedemann-Franz law satisfied in any of the limiting cases? Explain.

Hint: Integrals of the type appearing in Eqs. (2) and (3) can in general be evaluated only numerically. However, the leading behavior in the limiting cases can be extracted analytically in the following manner. (This technique can be thought of as a "Sommerfeld expansion" for an insulator.) In the case $k_B T \ll \Delta$ notice that the argument of cosh is always large meaning that cosh can be approximated by an exponential. The remaining integral is elementary. This is equivalent to replacing Fermi-Dirac distribution by Maxwell-Boltzmann. Think about why this is the right thing to do in the low-T regime. In the case $k_B T \gg \Delta$ it is convenient to write the integral as $\int_\Delta^\infty = \int_0^\infty - \int_0^\Delta$. The first integral can be evaluated exactly (with help of Mathematica or tables). In the second integral notice that the argument of cosh is always small and can be approximated by $\cosh(0) = 1$. The remaining integral is again elementary.

2. (10 points) *"E-ph interaction in 1D"* Consider a one-dimensional system of electrons interacting with phonons according to the standard Frölich Hamiltonian,

$$H = \sum_k \epsilon_k c_k^\dagger c_k + \sum_q \hbar\omega_q a_q^\dagger a_q + M \sum_{k,q} (a_{-q}^\dagger + a_q) c_k^\dagger c_{k-q},$$

with $\hbar\omega_q = W|\sin(qa/2)|$. The lattice, originally of spacing a, has become dimerized by the e-ph interaction so that period is now $2a$. A gap has consequently appeared in the electron band structure at $k = \pi/2a$ and the energy dispersion of the two bands is

$$\epsilon_k = \pm[A + B\cos(2ka)],$$

with A and B both positive and $A - B \gg W > 0$. Consider the case of one electron per atom, i.e. the lower band completely filled. The matrix element M is a constant and $M^2 = G/N$, with N the number of atoms. Find the condition on the magnitude G in terms of W, A, and B in order for the phonon energy at $q = \pi/a$ to be reduced to zero. Interpret this result physically.