PHYS 412 – Heat capacity of a metal, project guidelines and deliverables – Fall 2017

Guidelines:

As we have discussed in the course, the heat capacity of a metal can be attributed to two contributions, the free charge carriers (electrons) and the lattice (phonons), which can be modeled by the quantum free electron (QFE) and Debye models, respectively. For the QFE model, the heat capacity of the lattice at constant volume is given by:

$$C_V = \left(\frac{\partial\langle E\rangle}{\partial T}\right)_V = \int_0^{\infty} E\, g(E)\frac{\partial f(E)}{\partial T}\, dE$$

where E is given by the free-electron energy, $g(E)$ is the QFE density of states, and $f(E)$ is the Fermi-Dirac distribution. For the Debye model, the molar heat capacity of the lattice is given by the temperature derivative of Eq. 4.44 in Hofmann, which is (see pg. 60 from Hook and Hall as well as our lecture notes):

$$C_V = \left(\frac{\partial\langle E\rangle}{\partial T}\right)_V = 9N_A k_B \left(\frac{T}{\Theta_D}\right)^3 \int_0^{\Theta_D/T} \frac{x^4 e^x}{(e^x - 1)^2}\, dx$$

where the dimensionless parameter $x = \hbar\omega/k_B T$ and the Debye temperature $\Theta_D = \hbar\omega_D/k_B$.

In this project, you will write computer code to calculate each contribution using the full integral expressions for the QFE and Debye, and the total heat capacity which is simply the sum of the two contributions. The objectives are:

1. First determine the Fermi temperature T_F for the electrons and Debye temperature Θ_D for the phonons for an unknown material (data provided), by fitting experimental data in a plot of C_V/T vs. T^2 and using the low temperature approximations we developed in the course.

2. Using your values for T_F and Θ_D, calculate and graph the heat capacity for electrons and phonons using the full integral expressions. Confirm that they agree with the low temperature approximate expressions at low temperature, and determine the temperatures (in fractions T/T_F and T/Θ_D, respectively) at which the low temperature approximations are no longer good approximations to the full integral expressions, e.g. when there is a deviation greater than a percent.

3. Plot the full calculated heat capacity (sum of electron and phonon contributions) for the unknown metal on the same graph with the experimental heat capacity to test how well the models do in describing the experimental data.

Deliverables:

1. The code you wrote (submitted electronically, e.g. by email). Your code should have a simple method for changing the characteristics temperatures T_F and Θ_D in the model.

2. Write a 2-3 page report summarizing your observations. The report should include graphs for the objectives above. Include a discussion in the context of the theoretical models that explains your observations, including how well the models agree with the experimental data.