Assignments to Condensed Matter Theory I
Sheet 9

G. Cuniberti (Phy 4.1.29) Room H35
A. Donarini (Phy 3.1.24) Mon 03.07 (h 10.15)

sheet online: `http://www-MCG.uni-R.de/teaching/`

Problem set: Specific heat of metals and semiconductors

When we introduced the second quantization for Fermions we also calculated (Sheet 4) the partition function for a set of non interacting electrons with generic dispersion relation ϵ_λ. Now we want to specialize our calculation to two given simple models: namely of free electron in a metal and electron-holes of an intrinsic semiconductor. In particular the calculation of the temperature dependence of the chemical potential and internal energy of the metal reveals how the thermodynamical properties of a metal are determined by electrons at the Fermi surface. On the other hand the presence of a gap between the valence and the conduction band of an intrinsic semiconductor implies that only the *classical* high energy tale of the Fermi distribution for the electron (holes) gas in the conduction (valence) band must be taken into account.[1]

9.1. Thermodynamics of a metal

Calculate the temperature dependence of the chemical potential and of the internal energy of a system of N free non relativistic fermions in the limit of small temperatures ($k_{\rm B}T \ll E_{\rm F}$). In steps:

(a) Refresh the definition and calculation of the grancanonical partition function for a fermionic system.

(b) Evaluate the grancanonical partition function for a set of free non relativistic fermions with dispersion relation of the form: $\epsilon_k = \frac{\hbar^2 k^2}{2m}$ (in 3D).

(c) Calculate the density of states for the fermionic system just introduced.
`Hint:` Remember that we are in 3D and use spherical coordinates for a spherically symmetrical dispersion relation.

(d) The total number of particles in the system is the average of the particle number operator in the grancanonical ensemble. How can I write this number in terms of the Fermi distribution and the density of states?

(e) The chemical potential at zero temperature is the Fermi energy: can you prove this statement?
`Hint:` What is the form of the Fermi distribution at zero temperature? And what is the Fermi energy?

[1] As a guide in the solution of the present sheet we suggest to study paragraphs 4.8 and 4.9 of Czycholl, Theoretische Festkörperphysik, Springer, 2nd Edition (2004).

(f) The relation defined in point (d) defines implicitly the temperature dependence of the chemical potential. Explain why. Finally, calculate the low temperature dependence of the chemical potential making use of the Sommerfeld expansion.Note: See the already cited Czycholl's book for detailed explanations about the Sommerfeld expansion.

(g) The internal energy, $U(T)$, is the average energy of the system. Recall how this can be calculated starting from the grancanonical partition function. Express the internal energy as a function of the density of states and the Fermi distribution function and, making again use of the Sommerfeld expansion, calculate its low temperature dependence.

(h) How does the specific heat, $c_V = \frac{\partial U}{\partial T}$, of a metal depend on the temperature at very low temperatures?

(i) **[Kür]** The detailed calculation that you performed shows the linear dependence of the specific heat of a Fermi gas on the temperature at low temperatures. Could you guess this proportionality simply using the Pauli exclusion principle and the equipartition theorem (i.e. each electron considered as a classical particle should receive the same amount of average thermal energy $3/2k_{\mathrm{B}}T$)?

9.2. [Kür] Thermodynamics of a semiconductor

(a) Study the derivation of the specific heat for a semiconductor given at the pages 113-116 of the cited Czycholl's book and give the detail of the calculations leading from equation (4.200) to (4.202) of the text.

(b) Consider the following model of semiconductor with constant density of states for the valence and conduction band:

$$\mathrm{DOS}(E) = \begin{cases} \frac{1}{E_0} & \text{for } 0 < E < E_0 \text{ and } E_0 + \Delta < E < 2E_0 + \Delta \\ 0 & \text{elsewhere} \end{cases}$$

Assume that the chemical potential lies well inside the gap and calculate for this model the temperature dependence of the of the specific heat in the limit of small temperatures.