UiO : University of Oslo

FYS3400: Spring 2021

Module III: Obligatory assignment

Electrons I (FEG)

1. Implications of the Fermi-Dirac distribution (f_{FD}) on the energies (ϵ) reachable by the FEFG in 3D, and the magnitude of the chemical potential (μ).

   (a) Show that $\mu = \epsilon_{\mathrm{F}}$ at $T = 0$ K in the in FEFG model. Tips: Recall that, at $T = 0$ K, the Gibbs energy $G = N\mu$, where N is the number of particles; on the other hand, at $T = 0$ K, this expression may be compared with $G = E + pV$, where E, p and V are the total energy, pressure and volume of the system. E at $T = 0$ K can then be readily calculated by integrating $\mathrm{DOS}(\epsilon) \cdot f_{\mathrm{FD}} \cdot \epsilon$. Further, calculate the pressure by choosing an appropriate thermodynamic relation, e.g., $p = -(\partial E/\partial V)$; the anticipated result is $N\mu = E + pV = N\epsilon_{\mathrm{F}}$, i.e. $\mu = \epsilon_{\mathrm{F}}$.

   (b) Further, assume that this FEFG is heated up to $T > 0$ K. Continue assuming that $\mu = \epsilon_{\mathrm{F}}$, i.e., not changing with T. Plot f_{FD} as a function of $\epsilon/\epsilon_{\mathrm{F}}$ for $T = 0.01\ T_{\mathrm{F}}$, 0.1 T_{F}, 0.5 T_{F}, 1.0 T_{F} and 1.2 T_{F}. Compare the result with literature data, e.g., Fig. 3 on p.136 in Kittel. Up to what temperatures, approximately, is the assumption of $\mu = \epsilon_{\mathrm{F}}$ reasonable?

   (c) Now investigate the true temperature dependence of μ and plot $\mu/\epsilon_{\mathrm{F}}$ as a function of T/T_{F}. Tips: Remember that the total number of FEFG particles (N) is not changing with temperature. In other words, the integral of DOS at $T = 0$ K (see Eqs. 19 and 20 on p.140 in Kittel) and the integral of DOS$\cdot f_{\mathrm{FD}}$ at $T > 0$ K are both equal to N; from here it only remains to evaluate the integral of DOS$\cdot f_{\mathrm{FD}}$ numerically, and to plot $\mu/\epsilon_{\mathrm{F}}$ as a function of T/T_{F}.

   (d) Replot f_{FD} as a function of $\epsilon/\epsilon_{\mathrm{F}}$ for $T = 0.01\ T_{\mathrm{F}}$, 0.1 T_{F}, 0.5 T_{F}, 1.0 T_{F} and 1.2 T_{F} using the μ values found in part (c).

   (e) Make an estimate for the electronic heat capacity, taking into account that only a fraction of the electrons – those in the vicinity of ϵ_{F} – may contribute to an increase in the total energy due to heating. Explain why.

Electrons II (FEFG)

1. Solve the time-independent Schrödinger equation (TISE) using a potential energy in the form of a delta function having a magnitude of V_0 between the atomic sites of a 1D periodic lattice, as shown in Fig. 1 below (often referred as Kronig-Penney model in the literature). Illustrate, e.g., using a graph, that the discontinuities in the solution correlate with the idea of forbidden energy states. Further, using this solution, investigate limits of $V_0 = 0$ and $V_0 \to \infty$.

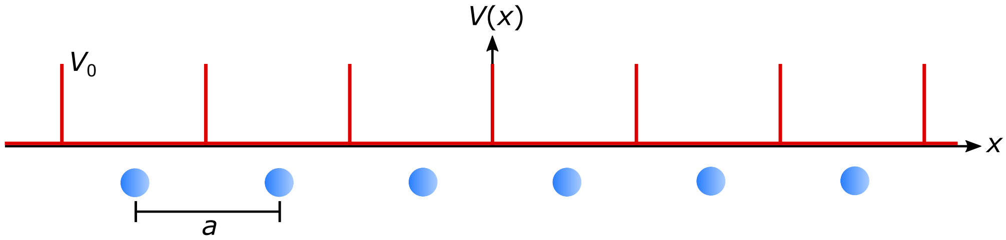

Figure 1: Potential consisting of delta functions with magnitude V_0.

Disordered systems (Relaxation of energy)

1. The DOS for TLS is:

$$gTLS(E) \approx \frac{P_0}{2} ln(4t_0/\tau_{min}(E))$$

   (a) Explain that this gives a time-dependent heat capacity $C(t_0) = Aln(4t_0/\tau_{min})$ where t_0 is the measurement time and A is some constant.

   (b) Use this to explain the time dependence of the released power $\dot{q} \sim 1/t_0$ as observed in the experimental results below. (Hint: assume good thermal contact to the reservior, so that all energy stored in TLS with $\tau < t_0$ is equilibrated at each time).

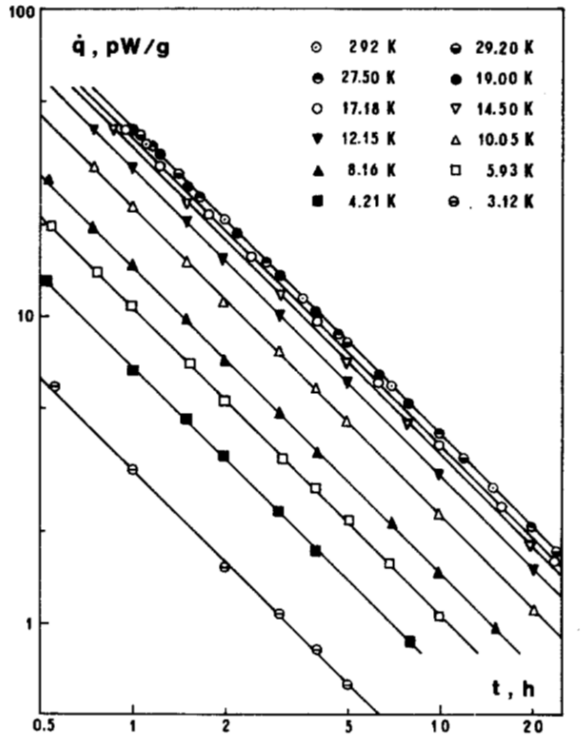

Fig. 2. The specific power released in specimen I ($Fe_{80}B_{14}Si_6$) after cooling from various T_1 ($3.12 \leqslant T_1 \leqslant 292$ K) to $T_0 = 1.3$ K, as a function of the time. Straight lines: $\dot{q} \sim t^{-1}$.