

Homework 5 Solutions

(1) Kinetic Energy of Sommerfeld-Fermi Electron Gas

The mean energy is, $\langle U \rangle = \int_0^\infty 2 \cdot D(U) U f_{FD}(U) dU$

where $f_{FD}(U) = \frac{1}{e^{(U-U_F)/k_B T} + 1} \rightarrow \theta(U_F - U)$ as $T \rightarrow 0$

and in three dimensions $D(U) = \frac{V}{(2)^{1/2} \pi^2} \left(\frac{m}{\hbar^2} \right)^{3/2} U^{1/2}$

So

$$\langle U \rangle = \int_0^\infty 2 \cdot D(U) U \theta(U) \theta(U_F - U) dU = \int_0^{U_F} \frac{V}{(2)^{1/2} \pi^2} \left(\frac{m}{\hbar^2} \right)^{3/2} U^{3/2} dU = \frac{V}{(2)^{1/2} \pi^2} \left(\frac{m}{\hbar^2} \right)^{3/2} \frac{U_F^{5/2}}{5/2}$$

But from definition of $U_F = \frac{\hbar^2}{2m} \left(\frac{3\pi^2 N}{V} \right)^{2/3}$, or by re-arrangement $\left(\frac{2mU_F}{\hbar^2} \right)^{3/2} = \frac{3\pi^2 N}{V}$.

Finally,
$$\langle U \rangle = \frac{V}{2\pi^2} \frac{3\pi^2 N}{V} \frac{2}{5} U_F = \frac{3}{5} N U_F$$

(2) Classical limit of Fermi gas.

(a) The classical limit corresponds to $(U - U_F) \gg k_B T$ (this will be proven below), so that $f_{FD} =$

$[\exp(U - U_F)/k_B T + 1]^{-1} \approx [\exp(U - U_F)/k_B T]^{-1} = \exp(U_F/k_B T) \exp(-U/k_B T)$ for any $U > 0$. Hence,

the mean energy is given by

$$\langle U \rangle \approx 2e^{U_F/k_B T} \int_0^\infty D(U) U e^{-U/k_B T} dU = \frac{(2)^{1/2} (m^* k_B T)^{5/2} V}{\pi^2 \hbar^3} e^{U_F/k_B T} \int_0^\infty (x)^{3/2} e^{-x} dx$$

The latter integral is evaluated as a Gamma function by the following identity from applied mathematics

$$\Gamma(n) = \int_0^\infty x^{n-1} e^{-x} dx$$

Thus we a mean specific energy:

$$\frac{\langle U \rangle}{V} = \frac{2(m^*)^{3/2} (k_B T)^{5/2} e^{U_F/k_B T}}{\sqrt{2} \pi^2 \hbar^3} \Gamma(5/2)$$

Two very useful evaluations of $\Gamma(n)$ are $\Gamma(3/2) = (\pi)^{1/2}/2$ and $\Gamma(5/2) = 3(\pi)^{1/2}/4$. Substitution of $\Gamma(5/2)$ results in

$$\frac{\langle U \rangle}{V} = \frac{3(m^*)^{3/2} (k_B T)^{5/2} e^{U_F/k_B T}}{2\sqrt{2} \pi^{3/2} \hbar^3} \quad (1)$$

To reduce this further we use the fact that the number of electrons is fixed in the Fermi model, and in the same classical approximation becomes

$$\langle N_e \rangle \approx 2e^{U_F/k_B T} \int_0^\infty D(U) e^{-U/k_B T} dU = \frac{(2)^{1/2} (m^* k_B T)^{3/2} V}{\pi^2 \hbar^3} e^{U_F/k_B T} \int_0^\infty (x)^{1/2} e^{-x} dx$$

Substitution of $\Gamma(3/2) = (\pi)^{1/2}/2$ results in

$$\frac{\langle N_e \rangle}{V} \equiv \rho \approx \frac{e^{U_F/k_B T}}{(2)^{1/2}} \left(\frac{m^* k_B T}{\pi \cdot \hbar^2} \right)^{3/2} \quad (2)$$

Substitution of this back into (1) yields

$$\frac{\langle U \rangle}{V} = \frac{3}{2} \frac{\langle N_e \rangle}{V} k_B T = \frac{3}{2} \rho \cdot k_B T \quad (3)$$

(b) From (2) we can write the following expression of U_F in terms of ρ , T , and m^* :

$$U_F \approx k_B T \cdot \ln \left[(2)^{1/2} \rho \left(\frac{\pi \hbar^2}{m^* k_B T} \right)^{3/2} \right] \quad (4)$$

Since $\ln(1) = 0$, the density that drives U_F to 0 is, for $m^* = m_e$,

$$\rho \approx \frac{1}{(2)^{1/2}} \left(\frac{m_e k_B \cdot 300}{\pi \cdot \hbar^2} \right)^{3/2} = 2.5 \times 10^{25} \text{ m}^{-3} = 2.5 \times 10^{19} \text{ cm}^{-3}$$

From (4), if the temperature is increased at this density, U_F has to go negative. The physical meaning of this is realized by recalling that the temperature-dependent Fermi energy is really the chemical potential μ . From the 1st law of thermodynamics, $\mu = \frac{\partial U}{\partial N}$, i.e., the change of energy with respect to change of particle number. So a negative U_F means that the addition of electrons to the Fermi gas (which would have to be done by an outside force) would *reduce the total energy*.

(c) From (3) we get $C_V \approx d\langle U \rangle/dT = (3/2) \langle N_e \rangle k_B$. This is just the electronic analog of the Dulong-Petit law for phonons, but a factor of two smaller. The factor of two can be explained by the classical law of equipartition: i.e., there is $(1/2)k_B T$ of energy per “degree-of-freedom”. In the case of electrons there are three degrees-of-freedom – three Cartesian components of the kinetic energy. For the phonons, there were six – three Cartesian components of the kinetic and potential energies.

(3) Chemical Potential in Two Dimensions

In general, $N = \int_0^\infty 2 \cdot D(U) f_{FD}(U) dU$, and $D(U) = \frac{dN(k)}{dk} \frac{dk}{dU} dU$

In two dimensions, $N(k) = \left(\frac{L}{2\pi}\right)^2 \pi k^2 = \frac{A}{4\pi} k^2 \Rightarrow \frac{dN(k)}{dk} = \frac{A}{2\pi} k$,

and from Fermi free electron energy relation, $k(\varepsilon) = \frac{\sqrt{2m\varepsilon}}{\hbar} \frac{1}{\hbar} \sqrt{\frac{m}{2\varepsilon}}$

So, $D(\varepsilon) = \frac{A}{\pi} \frac{\sqrt{2m\varepsilon}}{\hbar} \frac{1}{\hbar} \sqrt{\frac{m}{2\varepsilon}} = \frac{mA}{\pi\hbar^2}$ and $N = \int_0^\infty \frac{mA}{\pi\hbar^2} \left[\frac{dU}{e^{(U-U_F)/k_B T} + 1} \right]$

So let $z = e^{(U-U_F)/k_B T} + 1$, $dz = \frac{dU}{k_B T} e^{(U-U_F)/k_B T} = \frac{dU(z)}{k_B T}$

So, $N = \int_{\exp[-U_F/k_B T]}^\infty \left(\frac{mA}{\pi\hbar^2} \right) \frac{k_B T dz}{z(z+1)}$

From integral tables, $\int \frac{dz}{z(z+1)} = -\log \frac{1+z}{z}$

So, $N = \frac{mA k_B T}{\pi\hbar^2} \left[-\log\left(\frac{z+1}{z}\right) \right] \Big|_{\exp[-U_F/k_B T]}^\infty = \frac{mA k_B T}{\pi\hbar^2} \left[-\log(1) + \log\left(\frac{1+e^{-U_F/k_B T}}{e^{-U_F/k_B T}}\right) \right]$

And $N = \frac{mA k_B T}{\pi\hbar^2} \log\left(\frac{1+e^{-U_F/k_B T}}{e^{-U_F/k_B T}}\right) = \frac{mA k_B T}{\pi\hbar^2} \log\left(\frac{1+e^{U_F/k_B T}}{1}\right)$

And finally, $\exp\left(\frac{\pi\hbar^2 N}{mA k_B T}\right) = 1 + e^{U_F/k_B T} \Rightarrow U_F = k_B T \log\left[\exp\left(\frac{\pi\hbar^2 \rho_s}{mA k_B T}\right)\right]$

where ρ_s is the sheet density.

(4) Numerical Integration of Fermi Integrals. To do the thermodynamic calculations with the Sommerfeld-Fermi model at arbitrary temperatures, we must resort to the generic form of

$$\begin{aligned} \langle N_e \rangle &= \frac{2(m^*)^{3/2}V}{\sqrt{2}\pi^2\hbar^3} \int_0^\infty f_{FD}(U)U^{1/2}dU = \frac{2(m^*)^{3/2}(k_B T)^{3/2}V}{\sqrt{2}\pi^2\hbar^3} \int_0^\infty \frac{x^{1/2}}{\exp[x-x_F]+1}dx \\ &\equiv \frac{2(m^*)^{3/2}(k_B T)^{3/2}}{\sqrt{2}\pi^2\hbar^3} F_{1/2}(x_F) \end{aligned}$$

where $x \equiv U/k_B T$ and $x_F \equiv U_F/k_B T$, and

$$F_y(x_F) = \int_0^\infty \frac{x^y}{\exp[x-x_F]+1} dx$$

This is easy evaluate numerically in MATLAB using x_F as a parameter. Some results obtained with the `quadl.m` function in Matlab (Lobatto algorithm) are tabulated below and plotted in Figs 1 and 2 assuming $m^* = m_e$ and $T = 300$ K.

Table I		
x_F	$F_{1/2}(x_F)$	ρ [m^{-3}]
-20	1.75E-09	5.0E+16
-10	4.01E-05	1.1E+21
0	6.78E-01	1.9E+25
10	2.13E+01	6.0E+26
20	5.98E+01	1.7E+27
30	1.10E+02	3.1E+27
40	1.69E+02	4.8E+27
50	2.36E+02	6.7E+27
60	3.10E+02	8.8E+27
70	3.91E+02	1.1E+28
80	4.77E+02	1.4E+28
90	5.69E+02	1.6E+28
100	6.67E+02	1.9E+28

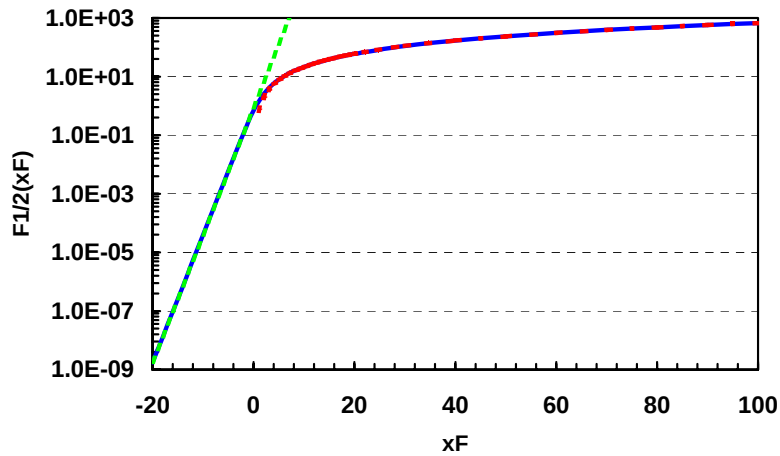


Fig. 1. Blue curve: numerical solution for the Fermi integral of order $1/2$. The dashed green and red lines are the low-temperature (degenerate) and high-temperature (non-degenerate) approximations, respectively. Notice how well the two approximations work except around $x_F = 0$.

Very important: Table I and Fig. 1 represent the numerical/graphical proofs of our earlier (assumed) definition of the classical (i.e., nondegenerate) limit of the Fermi gas: $f_{FD} \approx \exp(U_F/k_B T) \exp(-U/k_B T)$ for any $U > 0$. To make this clearer, Table II “zooms-in” on the values of x_F in the range $-10 < x_F < 10$ and lists the quantity $\exp(-x_F) \equiv \exp(-U_F/k_B T)$. Clearly this quantity is $\gg 1$ for $x_F < 0$ and $|x_F| \gg 1$, so that $\exp(U_F/k_B T) \exp(-U_F/k_B T)$ is also $\gg 1$ under the same conditions *since the energy is always defined positive for a Fermi gas (because there is kinetic energy only) and $\exp(U_F/k_B T) > 1$ for any positive U* . Hence, $f_{FD} = [\exp(U_F/k_B T) \exp(-U_F/k_B T) + 1]^{-1} \ll 1$, which is why this limit is called “nondegenerate”; i.e., the electrons are “not degenerated” into the same energy states. Clearly, the definition of this limit by the simple relation $x_F < 0$ and $|x_F| \gg 1$ is subtle. It is better stated by spelling out the definition of x , leading to $U_F < 0$ and $|U_F| \gg k_B T$. Clearly it is not enough just to say that $U_F < 0$ - a mistake sometimes made in semiconductor device engineering.

Table II	
x_F	$\exp(-x_F)$
-10	2.20E+04
-9	8.10E+03
-8	2.98E+03
-7	1.10E+03
-6	4.03E+02
-5	1.48E+02
-4	5.46E+01
-3	2.01E+01
-2	7.39E+00
-1	2.72E+00
0	1.00E+00
1	3.68E-01
2	1.35E-01
3	4.98E-02
4	1.83E-02
5	6.74E-03
6	2.48E-03
7	9.12E-04
8	3.35E-04
9	1.23E-04
10	4.54E-05

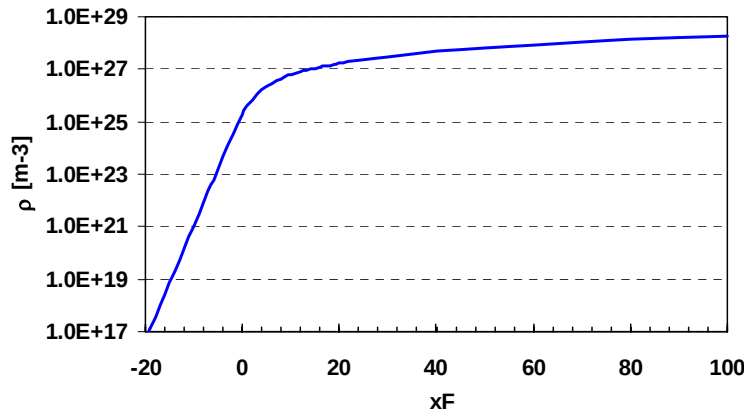


Fig. 2. Numerical solution to the carrier concentration over the range of x_F in Fig. 1 assuming $m^* = m_e$ and $T = 300$ K.

(5) Screening and plasmons

(a) In the notes we derived an expression for the Debye screening length of

$$\beta_D = [(\epsilon k_B T / e^2 \rho_0)]^{1/2}$$

to describe the length scale over which the free electron Fermi gas responds to a spatial variation in the electrostatic potential in the classical limit. β_D is very useful in the description of electrostatic effects in semiconductors, for example. Although we did not say it at the time, the Maxwell-Boltzmann distribution of velocities discussed in class is, indeed, the classical (i.e., “non-degenerate” limit) of the free-electron Fermi gas. In HW#2 we derived the variance of the velocity for the Maxwell-Boltzmann distribution $\langle(\Delta v)^2\rangle = 3k_B T/m$. From elementary probability theory, the “rms” value is just the square-root of the variance, so $v_{rms} = (3k_B T/m)^{1/2}$. In our discussion of long-wavelength plasma waves, we derived the circular plasma resonance frequency $\omega_p = [e^2 \rho_0 / m_e]^{1/2}$. The substitution of v_{rms} and ω_p into β_D yields the fascinating result:

$$\beta = \frac{v_{rms}}{(3)^{1/2} \omega_p}$$

(b) In a derivation similar to ours but done in terms of a dielectric function and in wave-vector space, a quantity similar to β_D can be derived for the response of the free-electron Fermi gas in the quantum (i.e., “degenerate”) limit [see Kittel, Chapter 10, “Electrostatic Screening” Section]. It is called the Thomas-Fermi screening length in honor of those who first derived it, and is given by $\beta_{TF} = (2\epsilon U_F / 3ne^2)^{1/2}$ [in MKS units; caution, Kittel derives it in CGS units]. Since the electron gas is assumed degenerate, we can approximate $U_F \approx U_{F0}$. In Notes#10 we derived an alternative metric – the Fermi velocity v_F – by the definition $U_{F0} \equiv (1/2)m(v_F)^2$. Substitution leads to $\beta_{TF} = v_{TF} (m/3ne^2)^{1/2}$, which when combined with the definition of ω_p leads to

$$\beta_{TF} = \frac{v_F}{(3)^{1/2} \omega_p}$$

another fascinating result and a great mnemonic tool for β_{TF} . Note that it has exactly the same (reciprocal) dependence on the plasma frequency as β_D , and a direct dependence on the characteristic velocity. For a “degenerate” Fermi gas, the characteristic velocity is v_F . For a “non-degenerate” Fermi gas it is $v_{rms} = (3k_B T/m)^{1/2}$.

(c) For engineering purposes it is useful to calculate the Fermi-gas quantities and their classical limits for important materials, such as GaAs and copper. These are listed in the Table below assuming for GaAs assume $n = 2.0 \times 10^{18} \text{ cm}^{-3}$, $\epsilon_r = 12.8$, $m^* = 0.067 m_e$; and for Cu $\rho = 8.4 \times 10^{22} \text{ cm}^{-3}$, $\epsilon_r = 1$, and $m^* = m_e$. The table has two purposes. First, it provides quantitative insight into how the electrons behave in all electronic materials, since GaAs is representative of many semiconductors and Cu is representative of many metals. Second, it indicates how much error is incurred by making incorrect assumptions, such as assuming a Debye screening length in a metal instead of the Thomas-Fermi screening length.

Table II		
Material	GaAs	Copper
Carrier concentration [$1/\text{cm}^3$]	$2.0\text{E}+18$	$8.4\text{E}+22$
Temperature [K]	300	300
Relative dielectric constant	12.8	1.0
Effective mass [m^*/m_e]	0.067	1.0
Circular plasma freq [1/s]	$8.6\text{E}+13$	$1.6\text{E}+16$
Linear plasma freq [1/s]	$1.4\text{E}+13$	$2.6\text{E}+15$
Maxwell-Boltzmann rms velocity [m/s]	$4.5\text{E}+05$	$1.2\text{E}+05$
Fermi energy [J]; [eV]	$1.4\text{E}-20$; 0.086	$1.1\text{E}-18$; 7.0
Fermi velocity [m/s]	$6.7\text{E}+05$	$1.6\text{E}+06$
Debye screening length [m]	$3.0\text{E}-09$	$4.1\text{E}-12$
T-F screening length [m]	$4.5\text{E}-09$	$5.5\text{E}-11$