Sommerfeld expansion

Use the Sommerfeld expansion to calculate the temperature dependence of the chemical potential/internal energy in one/two/ three dimensions at low temperature.

Evaluation of integrals of the form

$$\int_{-\infty}^{\infty} H(\epsilon) f(\epsilon, T) d\epsilon \qquad \text{with} \qquad f(\epsilon, T) = \frac{1}{e^{\frac{\epsilon-\mu}{k_B T}} + 1}$$

can be done approximately with the Sommerfeld expansion

$$\int_{-\infty}^{\infty} \frac{H(\epsilon)}{e^{\frac{\epsilon-\mu}{k_B T}} + 1} d\epsilon = \int_{-\infty}^{\mu} H(\epsilon) d\epsilon + \frac{\pi^2}{6} (k_B T)^2 H'(\mu) + O([k_B T]^4) + ... \tag{1}$$

Here $H'(\mu)$ denotes the derivative of $H(\epsilon)$ with respect to ϵ evaluated at $\epsilon = \mu$. For low temperatures the underlying series is remarkably convergent so that terms higher then second order can often be neglected. Furthermore it is convenient to set the lower limit of integration to $\epsilon = 0$ since the lowest energy state can be defined to be zero.

To calculate certain properties such as the internal energy for a free electron gas we further need the density of states in the given dimension (see table 1).

Table 1: Density of states and Fermi energy for free electrons in one, two and three dimensions (can be found here[1]).

	1D	2D	3D
Density of states	$D(E) = \frac{n}{2\sqrt{E_F E}}$	$D(E) = \frac{n}{E_F}$	$D(E) = \frac{3n}{2E_F^{3/2}}\sqrt{E}$
Fermi energy E_F	$E_F = \frac{\pi^2 \hbar^2 n^2}{8m}$	$E_F = \frac{\pi \hbar^2 n}{m}$	$E_F = \frac{\hbar^2}{2m}(3\pi^2 n)^{\frac{2}{3}}$

Temperature dependence of the chemical potential

The electron density is defined as

$$n = \int_{-\infty}^{\infty} D(E) f(E, T) dE \qquad \text{resp.} \qquad n = \int_{E=0}^{E_F} D(E) dE. \tag{2}$$

[1] `http://lamp.tu-graz.ac.at/~hadley/ss1/fermigas/electrontable/electrontable.html`

Using the Sommerfeld expansion with $H(E) = D(E)$ and omitting the terms $O([k_B T]^4)$ then gives

$$n = \int_0^{\mu} D(E)dE + \frac{\pi^2}{6}(k_B T)^2 \left(\frac{dD(E)}{dE}\right)_{E=\mu} \tag{3}$$

At low temperatures the chemical potential μ approaches the Fermi energy E_F with only small deviation. As the chemical potential is a function of T^2, the integral in equation (3) can be approximated by

$$\int_0^{\mu} H(E)dE \simeq \int_0^{E_F} H(E)dE + (\mu - E_F)H(E_F). \tag{4}$$

For the chemical potential μ in the last term of eq. (3) the Fermi energy E_F can be used in good approximation (the other terms would be already of order $O([k_B T]^4)$) which then results in the following expression:

Sommerfeld expansion

$$\int_0^{\infty} H(E)f(E,T)dE \simeq \int_0^{E_F} H(E)dE + (\mu - E_F)H(E_F) + \frac{\pi^2}{6}(k_B T)^2 \left. H'(E)\right|_{E=E_F} \tag{5}$$

Now the expressions for the chemical potential in one, two and three dimensions are derived:

1D

$$\begin{aligned} n &= \int_0^{\infty} \frac{n}{2\sqrt{E_F E}} f(E,T)dE \\ n &= \underbrace{\int_{E=0}^{E_F} D(E)dE}_{=n} + \frac{n}{2\sqrt{E_F}} \left((\mu - E_F)\frac{1}{\sqrt{E_F}} - \left. \frac{\pi^2}{12E^{3/2}}(k_B T)^2 \right|_{E=E_F} \right) \\ \frac{\mu - E_F}{E_F} &= \frac{\pi^2}{12E_F^2}(k_B T)^2 \\ \mu &= \underline{\underline{E_F + \frac{\pi^2}{12E_F}(k_B T)^2}} \end{aligned} \tag{6}$$

2D

$$\begin{aligned} n &= \int_0^{\infty} \frac{n}{\sqrt{E_F}} f(E,T)dE \\ n &= \underbrace{\int_{E=0}^{E_F} D(E)dE}_{=n} + (\mu - E_F)\frac{n}{\sqrt{E_F}} \\ \mu &= \underline{\underline{E_F}} \end{aligned} \tag{7}$$

3D

$$n = \int_0^\infty \frac{3n}{2E_F^{3/2}} \sqrt{E} f(E,T) dE$$

$$n = \underbrace{\int_{E=0}^{E_F} D(E) dE}_{=n} + \frac{3n}{2E_F^{3/2}} \left((\mu - E_F)\sqrt{E_F} + \frac{\pi^2}{12\sqrt{E}} (k_B T)^2 \bigg|_{E=E_F} \right)$$

$$\frac{\mu - E_F}{E_F^2} = \frac{\pi^2}{12 E_F^2} (k_B T)^2$$

$$\mu = E_F - \frac{\pi^2}{12 E_F} (k_B T)^2 \tag{8}$$

Temperature dependence of the internal energy

The internal energy is defined as

$$u = \int E D(E) f(E,T) dE. \tag{9}$$

Using the Sommerfeld expansion in the form eq. (5) with $H(E) = ED(E)$ and plugging in the density of states and the chemical potential gives:

1D

$$u = \int_0^\infty E \frac{n}{2\sqrt{E_F E}} f(E,T) dE =$$

$$= \frac{n}{2\sqrt{E_F}} \left(\int_{E=0}^{E_F} \sqrt{E} dE + (\mu - E_F) \frac{E_F}{\sqrt{E_F}} + \frac{\pi^2}{12\sqrt{E}} (k_B T)^2 \bigg|_{E=E_F} \right) =$$

$$= \frac{n}{2\sqrt{E_F}} \left(E^{3/2} \Big|_0^{E_F} + \frac{\pi^2}{12 E_F} (k_B T)^2 \frac{E_F}{\sqrt{E_F}} + \frac{\pi^2}{12\sqrt{E_F}} (k_B T)^2 \right) =$$

$$= \frac{n E_F}{3} + \frac{n\pi^2}{12 E_F} (k_B T)^2 \tag{10}$$

2D

$$u = \int_0^\infty E \frac{n}{E_F} f(E,T) dE = \frac{n}{2E_F} E^2 \Big|_0^{E_F} + \underbrace{(\mu - E_F)}_{=0} n + \frac{\pi^2}{6} (k_B T)^2 \frac{n}{E_F} \bigg|_{E=E_F} =$$

$$= \frac{n E_F}{2} + \frac{n\pi^2}{6 E_F} (k_B T)^2 \tag{11}$$

3D

$$
\begin{aligned}
u &= \int_0^\infty E \frac{3n}{2E_F^{3/2}} \sqrt{E} f(E,T) dE \\
&= \frac{3n}{2E_F^{3/2}} \left(\frac{2E^{5/2}}{5}\bigg|_0^{E_F} + (\mu - E_F)E_F^{3/2} + \frac{\pi^2}{6}(k_BT)^2 \, \frac{3}{2}\sqrt{E}\bigg|_{E=E_F} \right) = \\
&= \frac{3}{5} n E_F + \frac{3n}{2E_F^{3/2}} \left(-\frac{\pi^2}{12E_F}(k_BT)^2 E_F^{3/2} + \frac{\pi^2}{4}(k_BT)^2 \sqrt{E_F} \right) \\
&= \underline{\underline{\frac{3}{5} n E_F + \frac{n\pi^2}{4E_F}(k_BT)^2}}
\end{aligned} \tag{12}
$$

Bulk modulus, pressure, entropy, specific heat

Using the expression for the internal energy many other properties can be calculated easily. Table 2 gives an overview about their dependency on the internal energy.

Table 2: Expressions for the specific heat, entropy, Helmholtz free energy, pressure and bulk modulus as a function of the internal energy.

Specific heat	$c_V = \left(\frac{\partial u}{\partial T}\right)_{V=const.}$
Entropy	$s = \int \frac{C_V}{T} dT$
Helmholtz free energy	$f = u - Ts$
Pressure	$P = -\left.\frac{\partial F}{\partial V}\right\|_{N,T}$
Bulk modulus	$B = -V \frac{\partial P}{\partial V}$