

Sommerfeld formula
Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(November 01, 2018)

Arnold Johannes Wilhelm Sommerfeld: 5 December 1868 – 26 April 1951) was a German theoretical physicist who pioneered developments in atomic and quantum physics, and also educated and mentored a large number of students for the new era of theoretical physics. He served as doctoral supervisor for many Nobel Prize winners in physics and chemistry (only J. J. Thomson's record of mentorship is comparable to his). He introduced the 2nd quantum number (azimuthal quantum number) and the 4th quantum number (spin quantum number). He also introduced the fine-structure constant and pioneered X-ray wave theory.



https://en.wikipedia.org/wiki/Arnold_Sommerfeld

A Sommerfeld formula is an approximation method developed by Arnold Sommerfeld for the integrals represent statistical average using the Fermi-Dirac distribution.

$$\begin{aligned}\int_0^\infty f(\varepsilon)g(\varepsilon)d\varepsilon &= \int_0^\mu g(\varepsilon)d\varepsilon + \frac{\pi^2}{6\beta^2}g^{(1)}(\mu) + \frac{7\pi^4}{360\beta^4}g^{(3)}(\mu) \\ &+ \frac{31\pi^6}{15120\beta^6}g^{(5)}(\mu) + \frac{127\pi^8}{604800\beta^8}g^{(7)}(\mu) \\ &+ \frac{73\pi^{10}}{3421440\beta^{10}}g^{(9)}(\mu) + \frac{1414477\pi^{12}}{653837184000\beta^{12}}g^{(11)}(\mu) + \dots\end{aligned}$$

where $f(\varepsilon) = \frac{1}{e^{\beta(\varepsilon-\mu)} + 1}$ is the Fermi-Dirac distribution function. μ is the chemical potential. When $\beta\mu \gg 1$ (the condition of strong degeneracy), the derivative $-\frac{\partial f(\varepsilon)}{\partial \varepsilon}$ becomes a Dirac delta function, which takes a very sharp peak around $\varepsilon = \mu$. The chemical potential μ is dependent on temperature.

1. Derivation of Sommerfeld formula

We assume that

$$G(\varepsilon) = \int_0^\varepsilon g(x)dx$$

where $g(\varepsilon)$ is a slowly varying function around $\varepsilon = \mu$

$$g(\varepsilon) = G'(\varepsilon)$$

We now calculate the integral

$$\begin{aligned}I &= \int_0^\infty d\varepsilon f(\varepsilon)g(\varepsilon) \\ &= \int_0^\infty d\varepsilon f(\varepsilon)G'(\varepsilon) \\ &= [f(\varepsilon)G(\varepsilon)]_0^\infty - \int_0^\infty d\varepsilon \frac{\partial f(\varepsilon)}{\partial \varepsilon} G(\varepsilon) \\ &= \int_0^\infty d\varepsilon \left[-\frac{\partial f(\varepsilon)}{\partial \varepsilon}\right] G(\varepsilon)\end{aligned}$$

Note that $-\frac{\partial f(\varepsilon)}{\partial \varepsilon} \approx \delta(\varepsilon - \mu)$ which is the Dirac delta function having a very sharp peak at $\varepsilon = \mu$. We expand $G(\varepsilon)$ by using Taylor expansion around $\varepsilon = \mu$

$$G(\varepsilon) = G(\mu) + \frac{1}{1!}(\varepsilon - \mu)G^{(1)}(\mu) + \frac{1}{2!}(\varepsilon - \mu)^2 G^{(2)}(\mu) + \frac{1}{3!}(\varepsilon - \mu)^3 G^{(3)}(\mu) + \dots$$

Thus we get

$$\begin{aligned} \int_0^\infty d\varepsilon f(\varepsilon)g(\varepsilon) &= \int_0^\infty d\varepsilon \left[-\frac{\partial f(\varepsilon)}{\partial \varepsilon}\right] \left[G(\mu) + \frac{1}{1!}(\varepsilon - \mu)G^{(1)}(\mu) + \frac{1}{2!}(\varepsilon - \mu)^2 G^{(2)}(\mu) + \right. \\ &\quad \left. + \frac{1}{3!}(\varepsilon - \mu)^3 G^{(3)}(\mu) + \dots\right] \\ &= G(\mu) + \frac{1}{1!}G^{(1)}(\mu) \int_0^\infty d\varepsilon \left[-\frac{\partial f(\varepsilon)}{\partial \varepsilon}\right](\varepsilon - \mu) + \frac{1}{2!}G^{(2)}(\mu) \int_0^\infty d\varepsilon \left[-\frac{\partial f(\varepsilon)}{\partial \varepsilon}\right](\varepsilon - \mu)^2 \\ &\quad + \frac{1}{3!}G^{(3)}(\mu) \int_0^\infty d\varepsilon \left[-\frac{\partial f(\varepsilon)}{\partial \varepsilon}\right](\varepsilon - \mu)^3 + \dots \end{aligned}$$

We put $x = \beta(\varepsilon - \mu)$ with $\mu\beta \gg 1$.

$$G(\mu) = \int_0^\mu g(\varepsilon) d\varepsilon$$

$$G^{(1)}(\mu) = g(\mu), \quad G^{(2)}(\mu) = g^{(1)}(\mu), \quad G^{(3)}(\mu) = g^{(2)}(\mu), \dots$$

Then we have

$$\begin{aligned}
\int_0^{\infty} d\varepsilon f(\varepsilon)g(\varepsilon) &= \int_0^{\mu} g(\varepsilon)d\varepsilon + \frac{g(\mu)}{\beta} \int_{-\infty}^{\infty} dx \frac{x}{(e^x+1)(e^{-x}+1)} \\
&+ \frac{1}{2\beta^2} g^{(1)}(\mu) \int_{-\infty}^{\infty} dx \frac{x^2}{(e^x+1)(e^{-x}+1)} + \frac{1}{6\beta^3} g^{(2)}(\mu) \int_{-\infty}^{\infty} dx \frac{x^3}{(e^x+1)(e^{-x}+1)} \\
&+ \frac{1}{24\beta^4} g^{(3)}(\mu) \int_{-\infty}^{\infty} dx \frac{x^4}{(e^x+1)(e^{-x}+1)} + \frac{1}{120\beta^5} g^{(4)}(\mu) \int_{-\infty}^{\infty} dx \frac{x^5}{(e^x+1)(e^{-x}+1)} + \dots \\
&= \int_0^{\mu} g(\varepsilon)d\varepsilon + \frac{1}{2\beta^2} g^{(1)}(\mu) \int_{-\infty}^{\infty} dx \frac{x^2}{(e^x+1)(e^{-x}+1)} + \\
&+ \frac{1}{24\beta^4} g^{(3)}(\mu) \int_{-\infty}^{\infty} dx \frac{x^4}{(e^x+1)(e^{-x}+1)} + \dots
\end{aligned}$$

We have the Sommerfeld formula

$$\begin{aligned}
\int_0^{\infty} d\varepsilon f(\varepsilon)g(\varepsilon) &= \int_0^{\mu} g(\varepsilon)d\varepsilon + \frac{\pi^2}{6\beta^2} g^{(1)}(\mu) + \frac{7\pi^4}{360\beta^4} g^{(3)}(\mu) \\
&+ \frac{31\pi^6}{15120\beta^6} g^{(5)}(\mu) + \frac{127\pi^8}{604800\beta^8} g^{(7)}(\mu) \\
&+ \frac{73\pi^{10}}{3421440\beta^{10}} g^{(9)}(\mu) + \frac{1414477\pi^{12}}{653837184000\beta^{12}} g^{(11)}(\mu) + \dots
\end{aligned}$$

where

$$\begin{aligned}
\int_{-\infty}^{\infty} dx \frac{x^2}{(e^x+1)(e^{-x}+1)} &= \frac{\pi^2}{3}, & \int_{-\infty}^{\infty} dx \frac{x^4}{(e^x+1)(e^{-x}+1)} &= \frac{7\pi^4}{15} \\
\int_{-\infty}^{\infty} dx \frac{x^6}{(e^x+1)(e^{-x}+1)} &= \frac{31\pi^6}{21}, & \int_{-\infty}^{\infty} dx \frac{x^8}{(e^x+1)(e^{-x}+1)} &= \frac{127\pi^8}{15}
\end{aligned}$$

2. T dependence of the chemical potential

We start with

$$N = \int_0^{\infty} f(\varepsilon)D(\varepsilon)d\varepsilon$$

where

$$D(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \sqrt{\varepsilon} = a\sqrt{\varepsilon}$$

and

$$a = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2}$$

We get

$$\begin{aligned} N &= \int_0^\infty f(\varepsilon) D(\varepsilon) d\varepsilon \\ &\approx \int_0^\mu D(\varepsilon) d\varepsilon + \frac{\pi^2}{6} k_B^2 T^2 D'(\mu) \\ &= \frac{2a}{3} \mu^{3/2} + \frac{\pi^2}{6} k_B^2 T^2 \frac{a}{2\sqrt{\mu}} \end{aligned}$$

But we also have $\varepsilon_F = \mu(T=0)$. Then we have

$$N = \int_0^{\varepsilon_F} D(\varepsilon) d\varepsilon = \frac{2a}{3} \varepsilon_F^{3/2}.$$

Thus the chemical potential is given by

$$\frac{2a}{3} \varepsilon_F^{3/2} = \frac{2a}{3} \mu^{3/2} + \frac{\pi^2}{6} k_B^2 T^2 \frac{a}{2\sqrt{\mu}},$$

or

$$1 = \left(\frac{\mu}{\varepsilon_F} \right)^{3/2} + \frac{\pi^2}{8} \left(\frac{k_B T}{\varepsilon_F} \right)^2 \left(\frac{\mu}{\varepsilon_F} \right)^{-1/2}.$$

which is valid for the order of $\left(\frac{k_B T}{\varepsilon_F} \right)^2$ in the above expansion formula.

$$\left(\frac{\mu}{\varepsilon_F} \right)^{3/2} = 1 - \frac{\pi^2}{8} \left(\frac{k_B T}{\varepsilon_F} \right)^2 \left(\frac{\mu}{\varepsilon_F} \right)^{-1/2} \approx 1 - \frac{\pi^2}{8} \left(\frac{k_B T}{\varepsilon_F} \right)^2$$

or

$$\left(\frac{\mu}{\varepsilon_F}\right) \approx \left[1 - \frac{\pi^2}{8} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right]^{2/3} = 1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2$$

The chemical potential μ is approximated by the forms

$$\mu = \varepsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right] \quad (3D \text{ case})$$

This result confirms that the chemical potential (Fermi level) remains close to the Fermi energy as long as $k_B T \ll \varepsilon_F$. As the temperature increases, the chemical potential falls below the Fermi energy by a margin that grows quadratically with the temperature.

For the 1D case, similarly we have

$$\mu = \varepsilon_F \left[1 + \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right] \quad (1D \text{ case})$$

3. Total energy and specific heat

Using the Sommerfeld's formula, the total energy U of the electrons is approximated by

$$\begin{aligned} U &= \int_0^\infty f(\varepsilon) \varepsilon D(\varepsilon) d\varepsilon \\ &= \int_0^\mu \varepsilon D(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 [D(\varepsilon_F)] + \varepsilon_F D'(\varepsilon_F) \\ &= \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon + (\mu - \varepsilon_F) \varepsilon_F D(\varepsilon_F) + \frac{1}{6} \pi^2 (k_B T)^2 [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)] \end{aligned}$$

The total number of electrons is also approximated by

$$\begin{aligned} N &= \int_0^\infty f(\varepsilon) D(\varepsilon) d\varepsilon \\ &= \int_0^\mu D(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 D'(\varepsilon_F) \\ &= \int_0^{\varepsilon_F} D(\varepsilon) d\varepsilon + (\mu - \varepsilon_F) D(\varepsilon_F) + \frac{1}{6} \pi^2 (k_B T)^2 D'(\varepsilon_F) \end{aligned}$$

Since $\partial N / \partial T = 0$ (N is independent of T), we have

$$\mu' D(\varepsilon_F) + \frac{1}{3} \pi^2 k_B^2 T D'(\varepsilon_F) \approx 0,$$

or

$$\mu' = -\frac{1}{3} \pi^2 k_B^2 T \frac{D'(\varepsilon_F)}{D(\varepsilon_F)}.$$

The internal energy U is

$$U = \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon + (\mu - \varepsilon_F) \varepsilon_F D(\varepsilon_F) + \frac{1}{6} \pi^2 (k_B T)^2 [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)]$$

The specific heat C_{el} is defined by

$$\begin{aligned} C_{el} &= \frac{dU}{dT} \\ &= \frac{1}{3} \pi^2 k_B^2 T [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)] + \mu' \varepsilon_F D(\varepsilon_F) \\ &= \frac{1}{3} \pi^2 k_B^2 T D(\varepsilon_F) + \varepsilon_F \left[\frac{1}{3} \pi^2 k_B^2 T D'(\varepsilon_F) + \mu' D(\varepsilon_F) \right] \end{aligned}$$

The second term is equal to zero. So we have the final form of the specific heat

$$C_{el} = \frac{1}{3} \pi^2 k_B^2 D(\varepsilon_F) T.$$

In the above expression of C_{el} , we assume that there are N electrons inside volume $V (= L^3)$. The specific heat per mol is given by

$$\frac{C_{el}}{N} N_A = \frac{1}{3} \pi^2 \frac{D(\varepsilon_F)}{N} N_A k_B^2 T = \frac{1}{3} \pi^2 D^A(\varepsilon_F) N_A k_B^2 T.$$

where N_A is the Avogadro number and $D^A(\varepsilon_F)$ [1/(eV at)] is the density of states per unit energy per unit atom. Note that

$$\frac{1}{3} \pi^2 N_A k_B^2 = 2.35715 \text{ mJ eV/K}^2.$$

The entropy S is obtained as follows.

$$C_{el} = T \frac{\partial S}{\partial T} = \frac{1}{3} \pi^2 k_B^2 D(\epsilon_F) T$$

or

$$\frac{\partial S}{\partial T} = \frac{1}{3} \pi^2 k_B^2 D(\epsilon_F)$$

Thus we have

$$S = \frac{1}{3} \pi^2 k_B^2 D(\epsilon_F) T$$

which is the same as the heat capacity.

((Note)) The heat capacity of free electron

$$\frac{D(\epsilon_F)}{N} = \frac{a \sqrt{\epsilon_F}}{\frac{2a}{3} \epsilon_F^{3/2}} = \frac{3}{2 \epsilon_F} = \frac{3}{2 k_B T_F}$$

The electronic heat capacity per mol is

$$\frac{1}{3} \pi^2 \frac{D(\epsilon_F)}{N} N_A k_B^2 T = \frac{1}{3} \pi^2 \frac{3}{2 k_B T_F} R k_B T = \frac{\pi^2}{2} R \frac{T}{T_F}$$

Then γ is related to $D^A(\epsilon_F)$ as

$$\gamma = \frac{1}{3} \pi^2 N_A k_B^2 D^A(\epsilon_F),$$

or

$$\gamma (\text{mJ/mol K}^2) = 2.35715 D^A(\epsilon_F). \quad (2)$$

We now give the physical interpretation for Eq.(1). When we heat the system from 0 K, not every electron gains an energy $k_B T$, but only those electrons in orbitals within an energy range $k_B T$ of the Fermi level are excited thermally. These electrons gain an energy of $k_B T$. Only a fraction of the order of $k_B T D(\epsilon_F)$ can be excited thermally. The total electronic thermal kinetic energy E is of the order of $(k_B T)^2 D(\epsilon_F)$. The specific heat C_{el} is on the order of $k_B^2 T D(\epsilon_F)$.

((Note))

For Pb,	$\gamma = 2.98,$	$D^A(\varepsilon_F) = 1.26/(\text{eV at})$
For Al	$\gamma = 1.35,$	$D^A(\varepsilon_F) = 0.57/(\text{eV at})$
For Cu	$\gamma = 0.695,$	$D^A(\varepsilon_F) = 0.29/(\text{eV at})$

Table	$\gamma(\text{mJ/mol K}^2)$		(H.P. Myers)
Na:	1.38	Ti:	3.35
K:	2.08	V:	9.26
Mg:	1.3	Cr:	1.4
Al:	1.35	Mn:	9.2
Pb:	2.98	Fe:	4.98
Cu:	0.70	Co:	4.73
Ag:	0.65	Ni:	7.02
Au:	0.73	Pt:	7.0

4. Grand potential Φ_G for free electrons with the use of Sommerfeld expansion

Using the formula for fermions,

$$\Phi_G = -\frac{2}{3} \frac{gVm^{3/2}}{\sqrt{2\pi^2\hbar^3}} \int_0^\infty \frac{\varepsilon^{3/2}}{e^{\beta(\varepsilon-\mu)} + 1} d\varepsilon$$

and

$$N = \frac{gVm^{3/2}}{\sqrt{2\pi^2\hbar^3}} \int_0^\infty \sqrt{\varepsilon} d\varepsilon \quad (\text{at } T = 0 \text{ K})$$

with $g = 2$ for spin 1/2, we get the ratio

$$\begin{aligned}
\frac{\Phi_G}{N} &= \left(-\frac{2}{3}\right) \frac{\int_0^\infty \frac{\varepsilon^{3/2}}{e^{\beta(\varepsilon-\mu)} + 1} d\varepsilon}{\int_0^{\varepsilon_F} \sqrt{\varepsilon} d\varepsilon} \\
&= \left(-\frac{2}{3}\right) \frac{\frac{2}{5} \mu^{5/2}}{\frac{2}{3} \varepsilon_F^{3/2}} \left[1 + \frac{5\pi^2}{8} \left(\frac{k_B T}{\mu}\right)^2\right] \\
&= -\frac{2}{5} \varepsilon_F \left(\frac{\mu}{\varepsilon_F}\right)^{5/2} \left[1 + \frac{5\pi^2}{8} \left(\frac{k_B T}{\mu}\right)^2\right] \\
&\approx -\frac{2}{5} \varepsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right]^{5/2} \left[1 + \frac{5\pi^2}{8} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right] \\
&= -\frac{2}{5} \varepsilon_F \left[1 - \frac{5\pi^2}{24} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right] \left[1 + \frac{5\pi^2}{8} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right]
\end{aligned}$$

or

$$\Phi_G = -\frac{2}{5} N \varepsilon_F \left[1 + \frac{5\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right]$$

where we use the Sommerfeld expansion

$$\int_0^\infty d\varepsilon \frac{g(\varepsilon)}{e^{\beta(\varepsilon-\mu)} + 1} = \int_0^\mu g(\varepsilon) d\varepsilon + \frac{\pi^2 (k_B T)^2}{6} g^{(1)}(\mu)$$

We note that

$$\Phi_G = -PV = -k_B T \ln Z_G = -\frac{2U}{3}$$

The internal energy is

$$U = -\frac{2}{3} \Phi_G = \frac{3}{5} \varepsilon_F \left[1 + \frac{5\pi^2}{12} \left(\frac{k_B T}{\varepsilon_F}\right)^2\right]$$

The entropy S is obtained by

$$S = - \left(\frac{\partial \Phi_G}{\partial T} \right)_{V, \mu} = N \frac{\pi^2 k_B^2 T}{3 \varepsilon_F}$$

5. Summary

(i) Internal energy U

$$\begin{aligned} U &= \int_0^{\infty} \varepsilon D(\varepsilon) f(\varepsilon) d\varepsilon \\ &= \int_0^{\infty} u(\varepsilon) f(\varepsilon) d\varepsilon \\ &= \int_0^{\mu} u(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 u'(\mu) \end{aligned}$$

or

$$U = \int_0^{\mu} u(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)]$$

where

$$u(\varepsilon) = \varepsilon D(\varepsilon), \quad u'(\varepsilon) = D(\varepsilon) + \varepsilon D'(\varepsilon)$$

(ii) Number N :

$$\begin{aligned} N &= \int_0^{\infty} D(\varepsilon) f(\varepsilon) d\varepsilon \\ &= \int_0^{\mu} D(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 D'(\mu) \end{aligned}$$

Since N is independent of T ,

$$0 = \mu' D(\mu) + \frac{\pi^2}{3} k_B^2 T D'(\varepsilon_F)$$

or

$$0 = \mu' D(\mu) + \frac{\pi^2}{3} k_B^2 T D'(\mu)$$

(iii) Heat capacity C:

$$\begin{aligned} C &= \frac{\partial U}{\partial T} \\ &= \mu' u(\mu) + \frac{\pi^2}{3} k_B^2 T u'(\mu) \\ &= \mu' \mu D(\mu) + \frac{\pi^2}{3} k_B^2 T [D(\mu) + \mu D'(\mu)] \\ &= \mu [\mu' D(\mu) + \frac{\pi^2}{3} k_B^2 T D'(\mu)] + \frac{\pi^2}{3} k_B^2 T D(\mu) \\ &= \frac{\pi^2}{3} k_B^2 T D(\mu) \end{aligned}$$

or

$$C = \gamma T$$

with

$$\gamma = \frac{\pi^2}{3} k_B^2 D(\varepsilon_F)$$

Note that

$$u(\mu) = \mu D(\mu) \qquad u'(\mu) = D(\mu) + \mu D'(\mu)$$

(vi) Grand potential Φ_G

$$\begin{aligned} \ln Z_G &= \int_0^\infty D(\varepsilon) \ln(1 + z e^{-\beta \varepsilon}) d\varepsilon \\ &= \beta \int_0^\infty \phi(\varepsilon) \frac{1}{\frac{1}{z} e^{\beta \varepsilon} + 1} d\varepsilon \\ &= \beta \int_0^\infty \phi(\varepsilon) f(\varepsilon) d\varepsilon \end{aligned}$$

where

$$\phi'(\varepsilon) = D(\varepsilon)$$

Thus we have

$$\begin{aligned}\Phi_G &= -k_B T \ln Z_G \\ &= -\int_0^\infty \phi(\varepsilon) f(\varepsilon) d\varepsilon \\ &= -\left[\int_0^\mu \phi(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 \phi'(\mu) \right]\end{aligned}$$

When

$$D(\varepsilon) = a\sqrt{\varepsilon}$$

we get

$$\phi(\varepsilon) = \int D(\varepsilon) d\varepsilon = \frac{2}{3} a \varepsilon^{3/2}$$

$$u(\varepsilon) = \varepsilon D(\varepsilon) = a \varepsilon^{3/2} = \frac{3}{2} \phi(\varepsilon)$$

The internal energy is

$$\begin{aligned}U &= \int_0^\mu u(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 u'(\mu) \\ &= \frac{3}{2} \left[\int_0^\mu \phi(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 \phi'(\mu) \right] \\ &= -\frac{3}{2} \Phi_G\end{aligned}$$

or

$$\Phi_G = -PV = -\frac{2}{3} U$$

6. Derivation of entropy S (by R. Kubo)

Here we show the method used by Kubo. This method is very instructive to students. The chemical potential can be derived as follows. We start with

$$N = \int_0^{\varepsilon_F} D(\varepsilon) d\varepsilon = \int_0^{\varepsilon_F} \phi'(\varepsilon) d\varepsilon = \phi(\varepsilon_F) \quad (1)$$

at $T = 0$ K, where $D(\varepsilon) = \phi'(\varepsilon)$.

$$N = \int_0^{\infty} f(\varepsilon) D(\varepsilon) d\varepsilon = \int_0^{\mu} D(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 D'(\varepsilon_F) \quad (2)$$

Subtracting Eq.(1) from Eq.(2), we get

$$\int_{\varepsilon_F}^{\mu} D(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 D'(\varepsilon_F) = 0$$

Noting that

$$\int_{\varepsilon_F}^{\mu} D(\varepsilon) d\varepsilon = D(\varepsilon_F)(\mu - \varepsilon_F)$$

we have

$$D(\varepsilon_F)(\mu - \varepsilon_F) + \frac{1}{6} \pi^2 (k_B T)^2 D'(\varepsilon_F) = 0$$

Then the chemical potential is obtained as

$$\begin{aligned} \mu - \varepsilon_F &= -\frac{\pi^2}{6} (k_B T)^2 \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} \\ &= -\frac{\pi^2}{6} (k_B T)^2 \left[\frac{d \ln D(\varepsilon)}{d\varepsilon} \right]_{\varepsilon=\varepsilon_F} \\ &= -\frac{\pi^2}{6} (k_B T)^2 \frac{\phi''(\varepsilon_F)}{\phi'(\varepsilon_F)} \end{aligned}$$

or

$$\mu = \varepsilon_F - \frac{\pi^2}{6} (k_B T)^2 \frac{\phi''(\varepsilon_F)}{\phi'(\varepsilon_F)}$$

where

$$\phi'(\varepsilon) = D(\varepsilon)$$

The internal energy:

$$\begin{aligned} U &= \int_0^{\infty} \varepsilon D(\varepsilon) f(\varepsilon) d\varepsilon \\ &= \int_0^{\mu} \varepsilon D(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 \frac{d}{d\varepsilon} [\varepsilon D(\varepsilon)]|_{\varepsilon=\varepsilon_F} \\ &= \int_0^{\mu} \varepsilon D(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)] \end{aligned}$$

Here we use the Taylor expansion

$$\int_0^{\mu} \varepsilon D(\varepsilon) d\varepsilon = \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon + (\mu - \varepsilon_F) \varepsilon_F D(\varepsilon_F)$$

Thus the internal energy can be rewritten as

$$\begin{aligned} U &= \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon + (\mu - \varepsilon_F) \varepsilon_F D(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)] \\ &= \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon - \frac{\pi^2}{6} (k_B T)^2 \varepsilon_F \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} D(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)] \\ &= \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon - \frac{\pi^2}{6} (k_B T)^2 \varepsilon_F D'(\varepsilon_F) + \frac{\pi^2}{6} (k_B T)^2 [D(\varepsilon_F) + \varepsilon_F D'(\varepsilon_F)] \\ &= \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 D(\varepsilon_F) \end{aligned}$$

or

$$\begin{aligned}
U &= \int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 \phi'(\varepsilon_F) \\
&= \varepsilon_F \phi(\varepsilon_F) - \int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 \phi'(\varepsilon_F)
\end{aligned}$$

where

$$\int_0^{\varepsilon_F} \varepsilon D(\varepsilon) d\varepsilon = \int_0^{\varepsilon_F} \varepsilon \phi'(\varepsilon) d\varepsilon = \varepsilon_F \phi(\varepsilon_F) - \int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon$$

The heat capacity:

$$C = \frac{dU}{dT} = \frac{\pi^2}{3} k_B^2 \phi'(\varepsilon_F) T = \frac{\pi^2}{3} k_B^2 D(\varepsilon_F) T$$

Note that $D(\varepsilon_F) k_B T$ is the number of particles which are in the softened edge in the vicinity of Fermi energy.

The grand potential:

$$\begin{aligned}
\ln Z_G &= \int_0^{\infty} D(\varepsilon) \ln(1 + z e^{-\beta \varepsilon}) d\varepsilon \\
&= \beta \int_0^{\infty} \phi(\varepsilon) \frac{1}{\frac{1}{z} e^{\beta \varepsilon} + 1} d\varepsilon \\
&= \beta \int_0^{\infty} \phi(\varepsilon) f(\varepsilon) d\varepsilon \\
&\approx \beta \left[\int_0^{\mu} \phi(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 \phi'(\mu) \right]
\end{aligned}$$

Using the Taylor expansion,

$$\int_0^{\mu} \phi(\varepsilon) d\varepsilon = \int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon + (\mu - \varepsilon_F) \phi(\varepsilon_F)$$

$$\begin{aligned}
\Phi_G &= -k_B T \ln Z_G \\
&= -\int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon - (\mu - \varepsilon_F) \phi(\varepsilon_F) - \frac{\pi^2}{6} (k_B T)^2 \phi'(\varepsilon_F) \\
&= -\int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 \left[\frac{\phi''(\varepsilon_F)}{\phi'(\varepsilon_F)} \phi(\varepsilon_F) - \phi'(\varepsilon_F) \right] \\
&= -\int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 \phi'(\varepsilon_F) \left\{ \frac{\phi''(\varepsilon_F) \phi(\varepsilon_F) - [\phi'(\varepsilon_F)]^2}{[\phi'(\varepsilon_F)]^2} \right\}
\end{aligned}$$

where

$$\mu - \varepsilon_F = -\frac{1}{6} \pi^2 (k_B T)^2 \frac{D'(\varepsilon_F)}{D(\varepsilon_F)} = -\frac{1}{6} \pi^2 (k_B T)^2 \frac{\phi''(\varepsilon_F)}{\phi'(\varepsilon_F)}$$

Thus we have

$$\begin{aligned}
PV &= -\Phi_G \\
&= \int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon - \frac{1}{6} \pi^2 (k_B T)^2 \phi'(\varepsilon_F) \left\{ \frac{\phi''(\varepsilon_F) \phi(\varepsilon_F) - [\phi'(\varepsilon_F)]^2}{[\phi'(\varepsilon_F)]^2} \right\}
\end{aligned}$$

using these expressions, the entropy can be obtained as follows.

$$\begin{aligned}
ST &= -\Phi_G + U - \mu N \\
&= \int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon - \frac{1}{6} \pi^2 (k_B T)^2 \phi'(\varepsilon_F) \left\{ \frac{\phi''(\varepsilon_F) \phi(\varepsilon_F) - [\phi'(\varepsilon_F)]^2}{[\phi'(\varepsilon_F)]^2} \right\} \\
&\quad + \varepsilon_F \phi(\varepsilon_F) - \int_0^{\varepsilon_F} \phi(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 \phi'(\varepsilon_F) \\
&\quad - \left[\varepsilon_F - \frac{1}{6} \pi^2 (k_B T)^2 \frac{\phi''(\varepsilon_F)}{\phi'(\varepsilon_F)} \right] \phi(\varepsilon_F) \\
&= \frac{1}{3} \pi^2 (k_B T)^2 \phi'(\varepsilon_F) \\
&= \frac{1}{3} \pi^2 (k_B T)^2 D(\varepsilon_F)
\end{aligned}$$

or

$$S = \frac{1}{3} \pi^2 k_B^2 T D(\varepsilon_F)$$

7. Grand potential

The Gibbs free energy:

$$G = \mu N = F + PV = U - ST + PV$$

The grand potential is given by

$$\Phi_G = -PV = U - ST - \mu N$$

Since

$$\begin{aligned} d\Phi_G &= d(U - ST - \mu N) \\ &= TdS - PdV + \mu dN - SdT - TdS - \mu dN - Nd\mu \\ &= -SdT - PdV - Nd\mu \end{aligned}$$

we have

$$N = -\left(\frac{\partial \Phi_G}{\partial \mu}\right)_{T,V}, \quad S = -\left(\frac{\partial \Phi_G}{\partial T}\right)_{V,\mu}$$

We now calculate the grand potential using the Sommerfeld formula,

$$\begin{aligned} \Phi_G &= -PV \\ &= -k_B T \ln Z_G \\ &= -k_B T \int_0^\infty D(\varepsilon) \ln(1 + ze^{-\beta\varepsilon}) d\varepsilon \\ &= -\int_0^\infty \phi(\varepsilon) \frac{1}{\frac{1}{z} e^{\beta\varepsilon} + 1} d\varepsilon \\ &= -\int_0^\infty \phi(\varepsilon) f(\varepsilon) d\varepsilon \end{aligned}$$

with

$$\phi'(\varepsilon) = D(\varepsilon), \quad f(\varepsilon) = \frac{1}{\frac{1}{z} e^{\beta\varepsilon} + 1} = \frac{1}{e^{\beta(\varepsilon - \mu)} + 1}$$

8. The derivation of S from the grand potential

The entropy S is given by

$$S = - \left(\frac{\partial \Phi_G}{\partial T} \right)_{V, \mu} = \int_0^\infty \phi(\varepsilon) \left(\frac{\partial f(\varepsilon)}{\partial T} \right)_\mu d\varepsilon$$

Noting that

$$\left(\frac{\partial f(\varepsilon)}{\partial T} \right)_\mu = - \left(\frac{\varepsilon - \mu}{T} \right) \frac{\partial f}{\partial \varepsilon}$$

ST can be rewritten as

$$\begin{aligned} TS &= - \int_0^\infty \phi(\varepsilon) (\varepsilon - \mu) \frac{\partial f}{\partial \mu} d\varepsilon \\ &= \int_0^\infty h(\varepsilon) f(\varepsilon) d\varepsilon \end{aligned}$$

where

$$h(\varepsilon) = \frac{\partial}{\partial \varepsilon} [(\varepsilon - \mu) \phi(\varepsilon)] = (\varepsilon - \mu) \phi'(\varepsilon) + \phi(\varepsilon)$$

and

$$h'(\varepsilon) = (\varepsilon - \mu) \phi''(\varepsilon) + 2\phi'(\varepsilon)$$

Using the Sommerfeld formula, we get

$$\begin{aligned} TS &= \int_0^\mu h(\varepsilon) d\varepsilon + \frac{\pi^2}{6} (k_B T)^2 h'(\mu) \\ &= \int_0^\mu h(\varepsilon) d\varepsilon + \frac{\pi^2}{3} (k_B T)^2 \phi'(\mu) \end{aligned}$$

Here we note that

$$\begin{aligned} \int_0^\mu h(\varepsilon) d\varepsilon &= \int_0^\mu h(\varepsilon) d\varepsilon \\ &= [\phi(\varepsilon)(\varepsilon - \mu)]_0^\mu \\ &= 0 \end{aligned}$$

Thus ST can be approximated as

$$TS \approx \frac{\pi^2}{3} (k_B T)^2 \phi'(\varepsilon_F) = \frac{\pi^2}{3} (k_B T)^2 D(\varepsilon_F)$$

The entropy S is

$$S = \frac{\pi^2}{3} k_B^2 T D(\varepsilon_F)$$

9. The derivation of the number N from the grand potential

The number N is expressed by

$$N = - \left(\frac{\partial \Phi_G}{\partial \mu} \right)_{T,V}$$

Note that

$$\begin{aligned} \left(\frac{\partial \Phi_G}{\partial \mu} \right)_{T,V} &= - \int_0^\infty \phi(\varepsilon) \left(\frac{\partial f(\varepsilon)}{\partial \mu} \right)_T d\varepsilon \\ &= \int_0^\infty \phi(\varepsilon) \frac{\partial f(\varepsilon)}{\partial \varepsilon} d\varepsilon \\ &= - \int_0^\infty \phi'(\varepsilon) f(\varepsilon) d\varepsilon \\ &= - \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon \end{aligned}$$

where

$$\left(\frac{\partial f(\varepsilon)}{\partial \mu} \right)_T = - \frac{\partial f(\varepsilon)}{\partial \varepsilon}$$

This leads to the results which is familiar to us,

$$N = \int_0^\infty D(\varepsilon) f(\varepsilon) d\varepsilon$$

10. Derivation of the entropy using the Maxwell's relation

From the thermodynamics, dG can be expressed as

$$\begin{aligned}
dG &= d(U - ST + PV) \\
&= TdS - PdV + \mu dN - SdT - TdS + PdV + VdP \\
&= -SdT + VdP + \mu dN
\end{aligned}$$

leading to the relations

$$S = -\left(\frac{\partial G}{\partial T}\right)_{P,N}, \quad V = \left(\frac{\partial G}{\partial P}\right)_{T,N}, \quad \mu = \left(\frac{\partial G}{\partial N}\right)_{T,P}$$

From these relations, the Maxwell's relation can be expressed by

$$\left(\frac{\partial \mu}{\partial T}\right)_{P,N} = -\left(\frac{\partial S}{\partial N}\right)_{P,T}$$

since

$$\begin{aligned}
\left(\frac{\partial \mu}{\partial T}\right)_{P,N} &= \left(\frac{\partial}{\partial T}\right)_{P,N} \left(\frac{\partial G}{\partial N}\right)_{T,P} = \left(\frac{\partial^2 G}{\partial T \partial N}\right)_P \\
\left(\frac{\partial S}{\partial N}\right)_{P,T} &= -\left(\frac{\partial}{\partial N}\right)_{P,T} \left(\frac{\partial G}{\partial T}\right)_{P,N} = -\left(\frac{\partial^2 G}{\partial N \partial T}\right)_P
\end{aligned}$$

Suppose that N depends only T and μ . We get

$$\begin{aligned}
\left(\frac{\partial \mu}{\partial T}\right)_N &= \frac{\partial(\mu, N)}{\partial(T, N)} \\
&= \frac{\frac{\partial(\mu, N)}{\partial(T, \mu)}}{\frac{\partial(T, N)}{\partial(T, \mu)}} \\
&= -\frac{\frac{\partial(N, \mu)}{\partial(T, \mu)}}{\frac{\partial(N, T)}{\partial(\mu, T)}} \\
&= -\frac{\left(\frac{\partial N}{\partial T}\right)_\mu}{\left(\frac{\partial N}{\partial \mu}\right)_T}
\end{aligned}$$

and

$$\begin{aligned}
 \left(\frac{\partial S}{\partial N} \right)_T &= \frac{\partial(S, T)}{\partial(N, T)} \\
 &= \frac{\frac{\partial(S, T)}{\partial(\mu, T)}}{\frac{\partial(N, T)}{\partial(\mu, T)}} \\
 &= \frac{\left(\frac{\partial S}{\partial \mu} \right)_T}{\left(\frac{\partial N}{\partial \mu} \right)_T}
 \end{aligned}$$

Thus we have the relation

$$\left(\frac{\partial S}{\partial \mu} \right)_T = \left(\frac{\partial N}{\partial T} \right)_\mu$$

Here we note that

$$N = \int_0^\mu D(\varepsilon) d\varepsilon + \frac{1}{6} \pi^2 (k_B T)^2 D'(\mu)$$

Then we get

$$\left(\frac{\partial N}{\partial \mu} \right)_T = D(\mu) + \frac{1}{6} \pi^2 (k_B T)^2 D''(\mu) \approx D(\varepsilon_F)$$

$$\left(\frac{\partial N}{\partial T} \right)_\mu = \frac{\pi^2}{3} k_B^2 T D'(\mu) = \frac{\pi^2}{3} k_B^2 T D'(\varepsilon_F)$$

(a) Chemical potential

Using the above relation, we have

$$\left(\frac{\partial \mu}{\partial T} \right)_N = - \frac{\left(\frac{\partial N}{\partial T} \right)_\mu}{\left(\frac{\partial N}{\partial \mu} \right)_T} = - \frac{\pi^2}{3} k_B^2 T \frac{D'(\varepsilon_F)}{D(\varepsilon_F)}$$

or

$$\mu = \varepsilon_F - \frac{\pi^2}{6} k_B^2 T^2 \frac{D'(\varepsilon_F)}{D(\varepsilon_F)}$$

(b) Entropy S

Using the above relation, we can calculate the entropy S as

$$\left(\frac{\partial S}{\partial \mu} \right)_T = \left(\frac{\partial N}{\partial T} \right)_\mu = \frac{\pi^2}{3} k_B^2 T D'(\mu)$$

The integration of this with respect to μ leads to

$$S = \frac{\pi^2}{3} k_B^2 T D(\mu) \approx \frac{\pi^2}{3} k_B^2 T D(\varepsilon_F)$$

11. Sommerfeld formula: 1D case

We consider the case of one-dimensional system.

$$N = \int_0^\infty d\varepsilon f(\varepsilon) D_1(\varepsilon) = \int_0^{\varepsilon_F} d\varepsilon D_1(\varepsilon)$$

where the density of the state for the 1D system is

$$D_1(\varepsilon) = \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \varepsilon^{-1/2}$$

since

$$D_1(\varepsilon) d\varepsilon = 2 \left(\frac{L}{2\pi} \right) 2dk = \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \frac{d\varepsilon}{\sqrt{\varepsilon}}$$

The factor 2 of $2dk$ comes from the even function of the 1D energy dispersion relation. We use the Sommerfeld formula

$$N = \int_0^\infty d\varepsilon f(\varepsilon) \varphi(\varepsilon) = \int_0^\mu d\varepsilon \varphi(\varepsilon) + \frac{\pi^2}{6} k_B^2 T^2 \varphi'(\mu)$$

where

$$\varphi(\varepsilon) = D_1(\varepsilon) = \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \varepsilon^{-1/2} = a_1 \varepsilon^{-1/2}$$

$$\frac{d\varphi(\varepsilon)}{d\varepsilon} = \frac{L}{\pi} \left(\frac{2m}{\hbar^2} \right)^{1/2} \left(-\frac{1}{2} \right) \varepsilon^{-3/2} = -\frac{1}{2} a_1 \varepsilon^{-3/2}$$

Thus we have

$$\begin{aligned} N &= a_1 \int_0^\mu d\varepsilon \varepsilon^{-1/2} d\varepsilon + \frac{\pi^2}{6} k_B^2 T^2 \left(-\frac{1}{2} a_1 \mu^{-3/2} \right) \\ &= 2a_1 \mu^{1/2} - \frac{\pi^2}{12} k_B^2 T^2 a_1 \mu^{-3/2} \end{aligned} \quad (1)$$

But we also have

$$N = \int_0^{\varepsilon_F} d\varepsilon D_1(\varepsilon) = a_1 \int_0^{\varepsilon_F} \varepsilon^{-1/2} d\varepsilon = 2a_1 \varepsilon_F^{1/2} \quad (2)$$

Combining Eqs.(1) and (2), we get

$$2a_1 \varepsilon_F^{1/2} = 2a_1 \mu^{1/2} - \frac{\pi^2}{12} k_B^2 T^2 a_1 \mu^{-3/2}$$

or

$$\mu^{1/2} = \varepsilon_F^{1/2} + \frac{\pi^2}{24} k_B^2 T^2 \mu^{-3/2}$$

Then the chemical potential μ is

$$\begin{aligned} \left(\frac{\mu}{\varepsilon_F} \right)^{1/2} &= 1 + \frac{\pi^2}{24} \frac{k_B^2 T^2}{\varepsilon_F^{1/2}} \mu^{-3/2} \\ &\approx 1 + \frac{\pi^2}{24} \frac{k_B^2 T^2}{\varepsilon_F^2} \end{aligned}$$

or

$$\frac{\mu}{\varepsilon_F} = \left(1 + \frac{\pi^2}{24} \frac{k_B^2 T^2}{\varepsilon_F^2} \right)^2 \approx 1 + \frac{\pi^2}{12} \frac{k_B^2 T^2}{\varepsilon_F^2}$$

We make a plot of the number distribution as a function of $x = \varepsilon / \varepsilon_F$

$$D(\varepsilon)f(\varepsilon) \propto \frac{1}{\sqrt{x}} \frac{1}{\exp\left[\frac{x}{\alpha} - \frac{1}{\alpha}\left(1 + \frac{\pi^2}{12}\alpha^2\right)\right] + 1}$$

where $\alpha = k_B T / \varepsilon_F$ is changed as a parameter. We choose $\alpha = 0.3$.

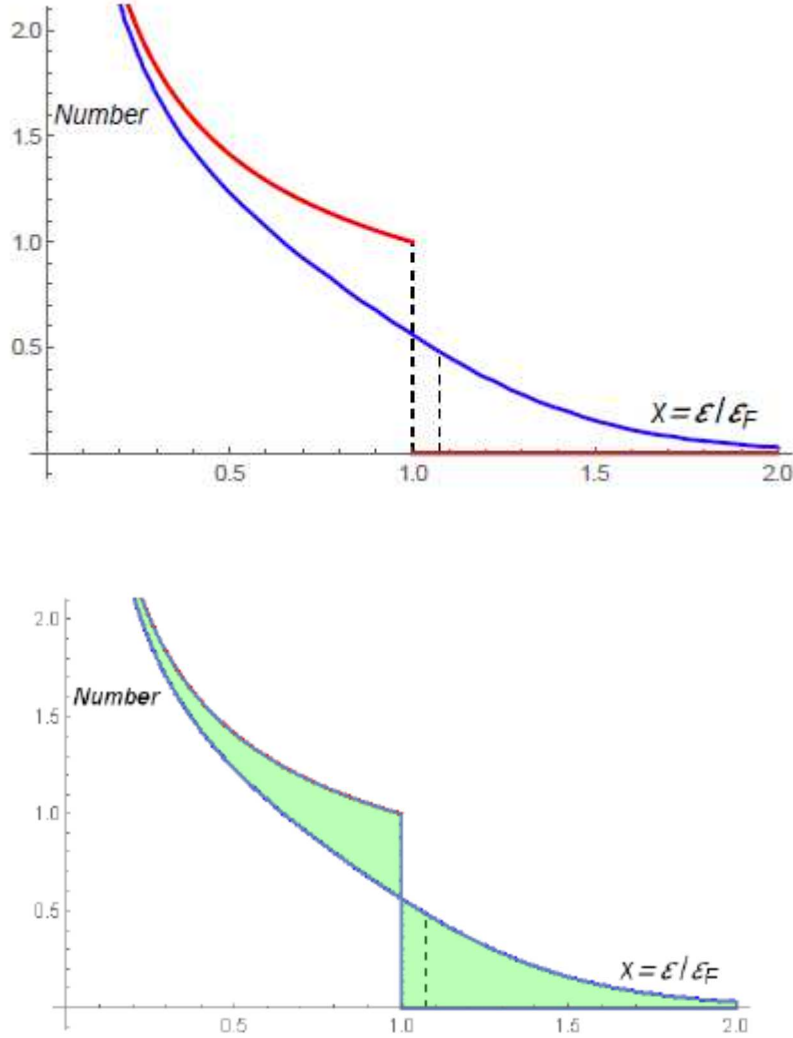
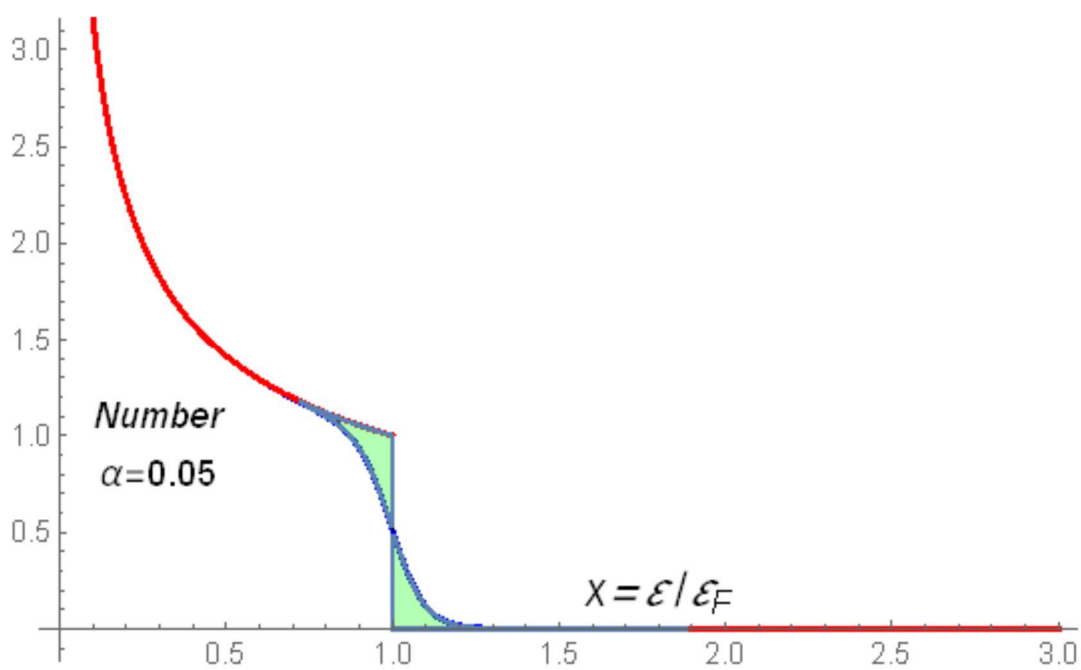
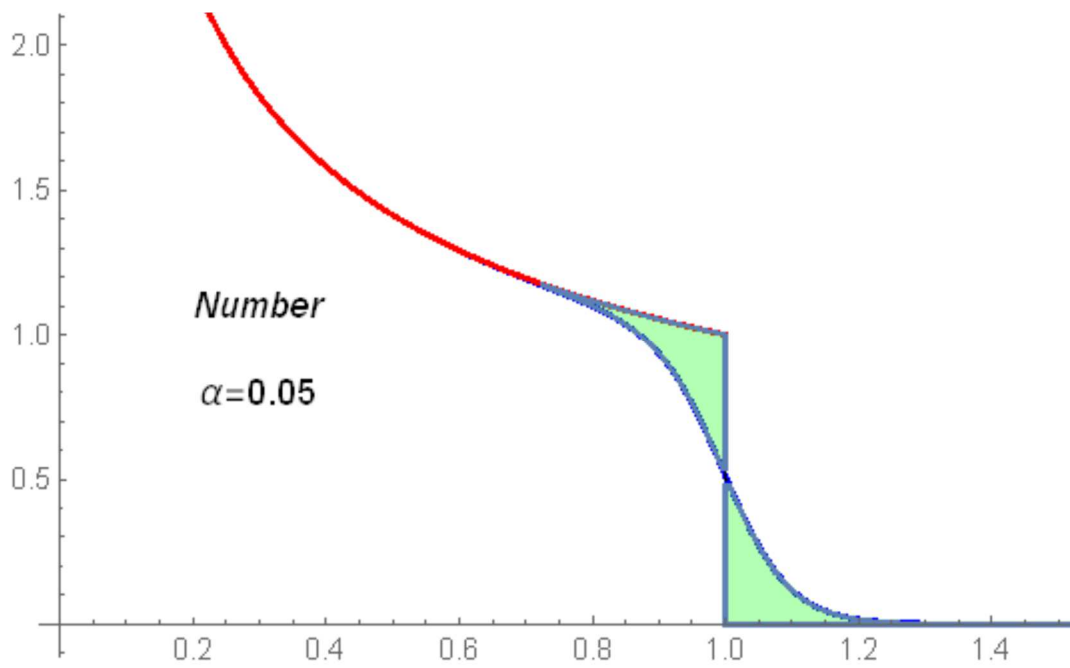
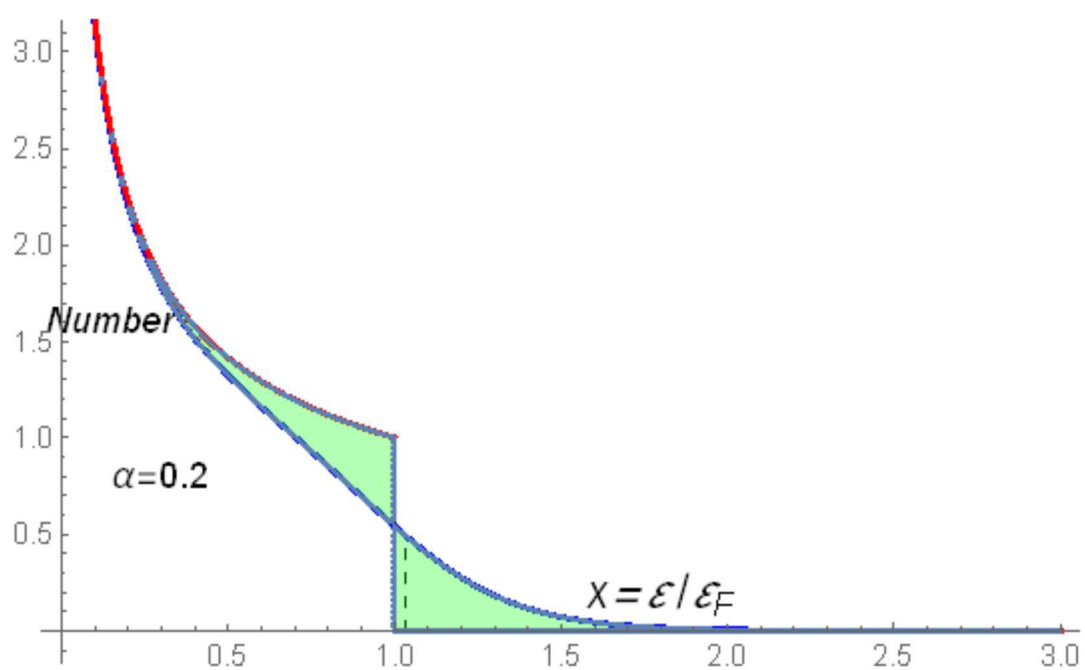
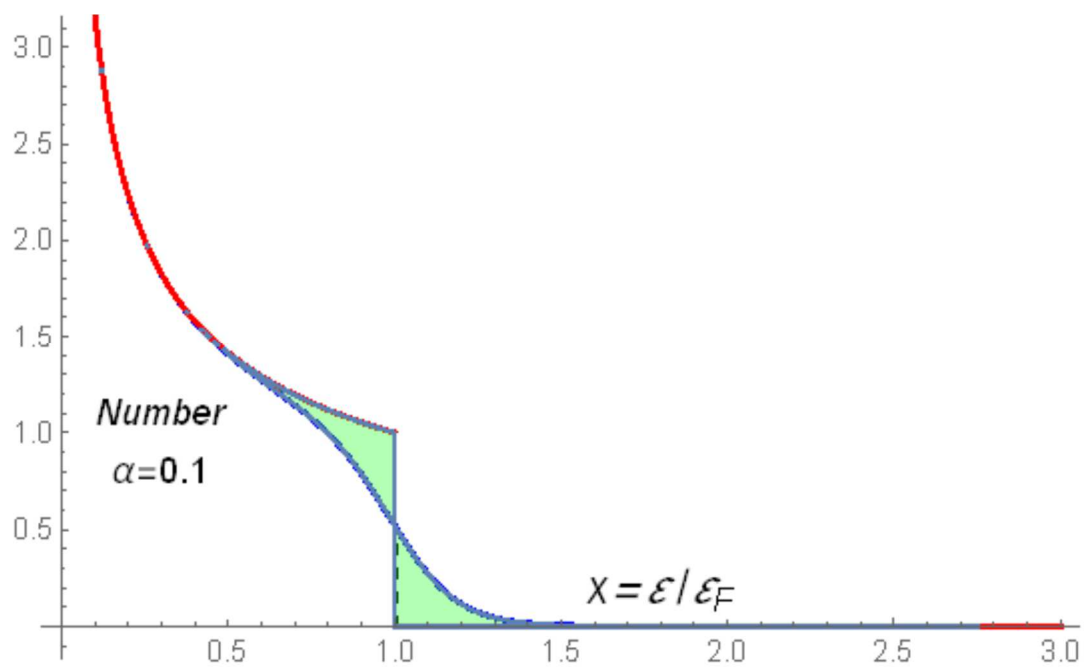
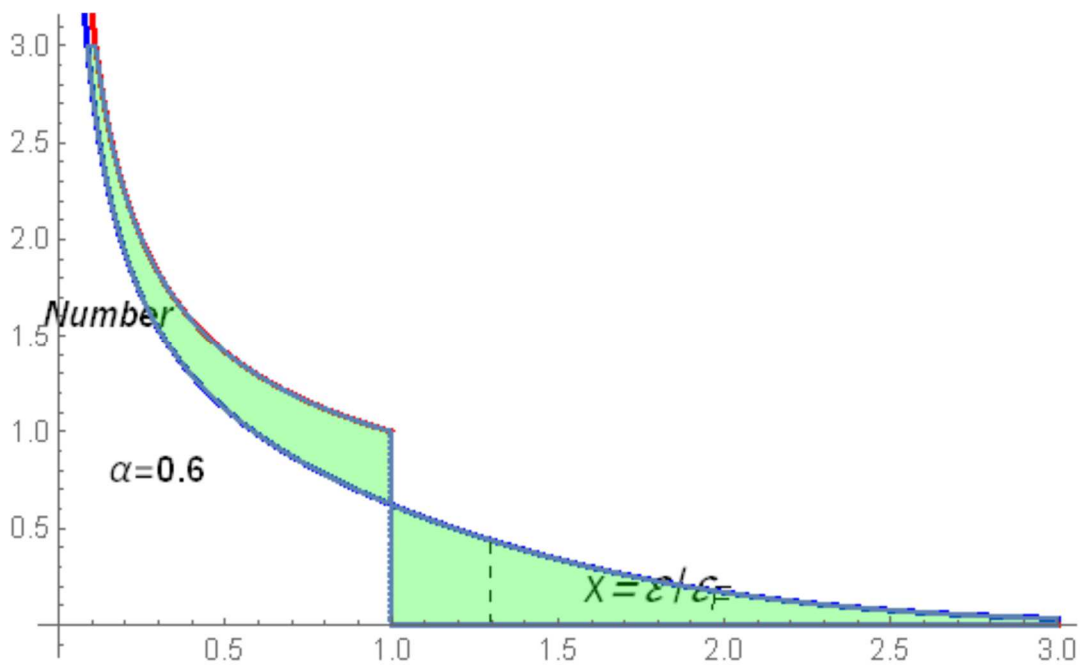
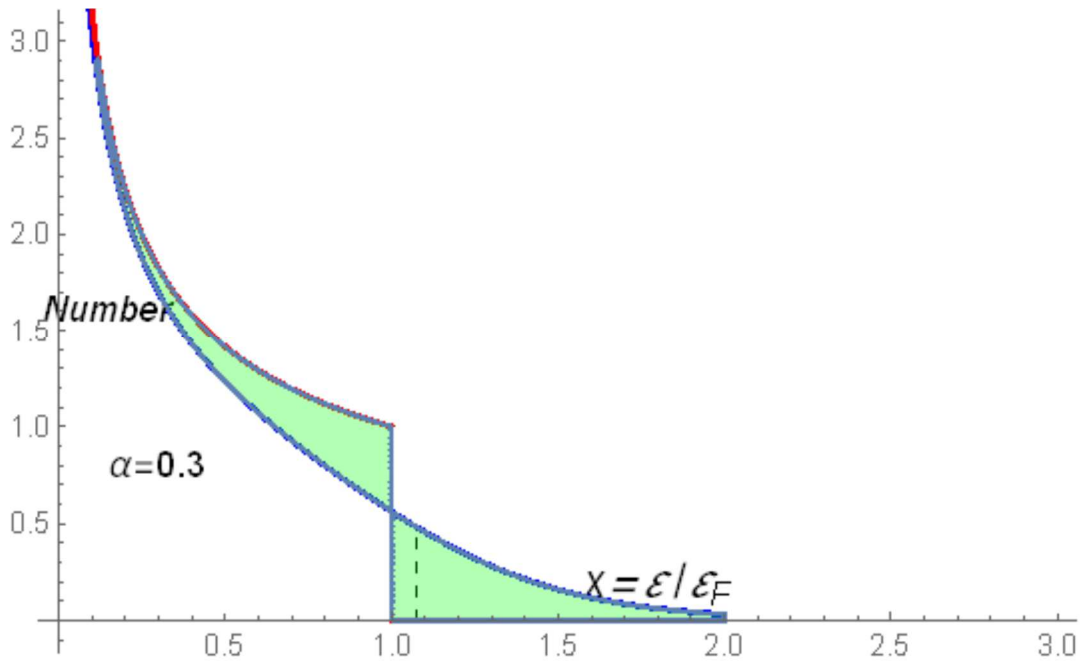


Fig. The number distribution vs $x = \varepsilon / \varepsilon_F$, $\alpha = k_B T / \varepsilon_F = 0.3$ for the 1D case. The chemical potential for the temperature with $\alpha = k_B T / \varepsilon_F = 0.3$ is denoted by the dashed line. It shifts to the high energy side from the Fermi energy at $T = 0$ K ($x = 1$). The area for $x > 1$ (shaded region denoted by green) is the same as the area below $x < 1$.







12. Sommerfeld formula for the 3D system

Next we consider the case of three-dimensional system.

$$N = \int_0^{\infty} d\epsilon f(\epsilon) D_3(\epsilon) = \int_0^{\epsilon_F} d\epsilon D_3(\epsilon) d\epsilon$$

where the density of states for the 3D system is

$$D_3(\varepsilon) = \frac{V}{2\pi^2} \left(\frac{2m}{\hbar^2} \right)^{3/2} \varepsilon^{1/2}$$

We use the Sommerfeld formula

$$N = \int_0^\infty d\varepsilon f(\varepsilon) \varphi(\varepsilon) = \int_0^\mu \varphi(\varepsilon) d\varepsilon + \frac{\pi^2}{6} k_B^2 T^2 \varphi'(\mu)$$

Thus we have

$$\begin{aligned} N &= a_3 \int_0^\mu \varepsilon^{1/2} d\varepsilon + \frac{\pi^2}{6} k_B^2 T^2 \frac{1}{2} a_3 \mu^{-1/2} \\ &= \frac{2}{3} a_3 \mu^{3/2} + \frac{\pi^2}{12} k_B^2 T^2 a_3 \mu^{-1/2} \end{aligned}$$

Combining Eqs.(1) and (2), we get

$$\frac{2}{3} a_3 \varepsilon_F^{3/2} = \frac{2}{3} a_3 \mu^{3/2} + \frac{\pi^2}{12} k_B^2 T^2 a_3 \mu^{-1/2}$$

or

$$\varepsilon_F^{3/2} = \mu^{3/2} + \frac{\pi^2}{8} k_B^2 T^2 \mu^{-1/2}$$

Then the chemical potential is

$$\begin{aligned} \left(\frac{\mu}{\varepsilon_F} \right)^{3/2} &= 1 - \frac{\pi^2}{8} k_B^2 T^2 \frac{\mu^{-1/2}}{\varepsilon_F^{3/2}} \\ &\approx 1 - \frac{\pi^2}{8} \frac{k_B^2 T^2}{\varepsilon_F^2} \end{aligned}$$

or

$$\left(\frac{\mu}{\varepsilon_F} \right) = \left(1 - \frac{\pi^2}{8} \frac{k_B^2 T^2}{\varepsilon_F^2} \right)^{2/3} \approx 1 - \frac{\pi^2}{12} \frac{k_B^2 T^2}{\varepsilon_F^2}$$

or

$$\mu = \varepsilon_F \left(1 - \frac{\pi^2}{12} \frac{k_B^2 T^2}{\varepsilon_F^2} \right)$$

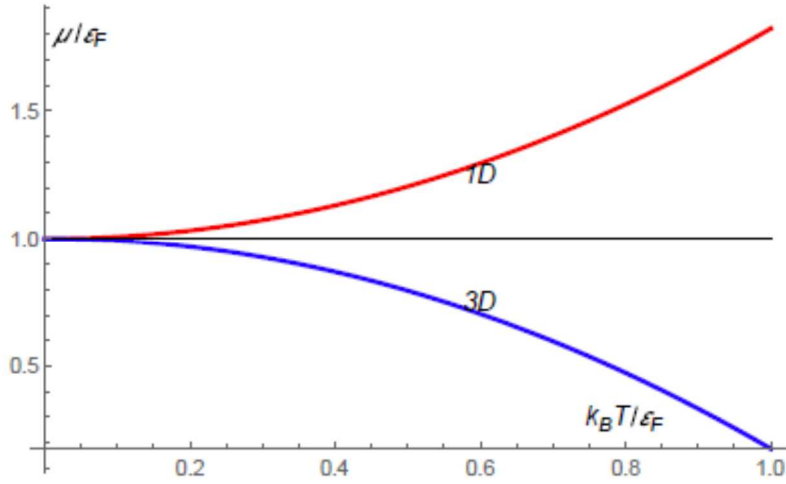
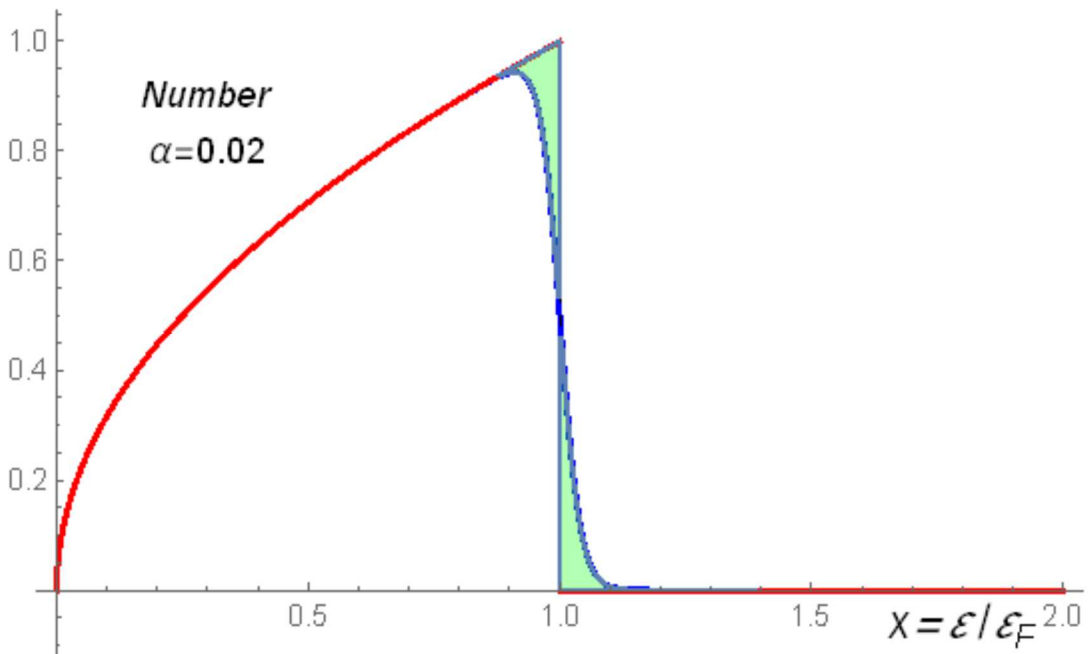
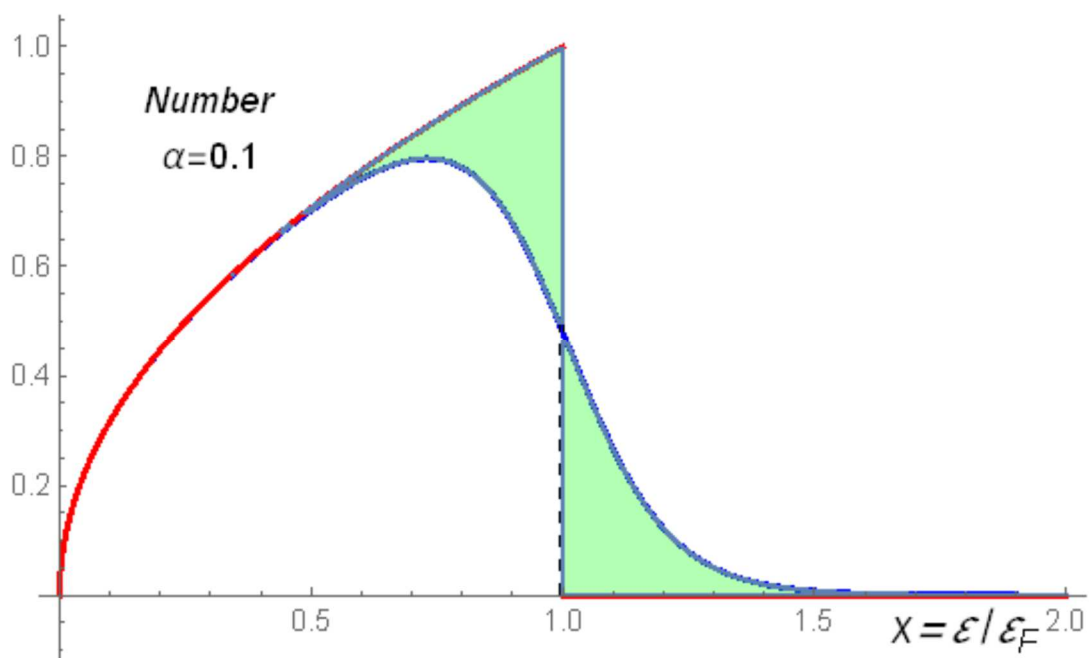
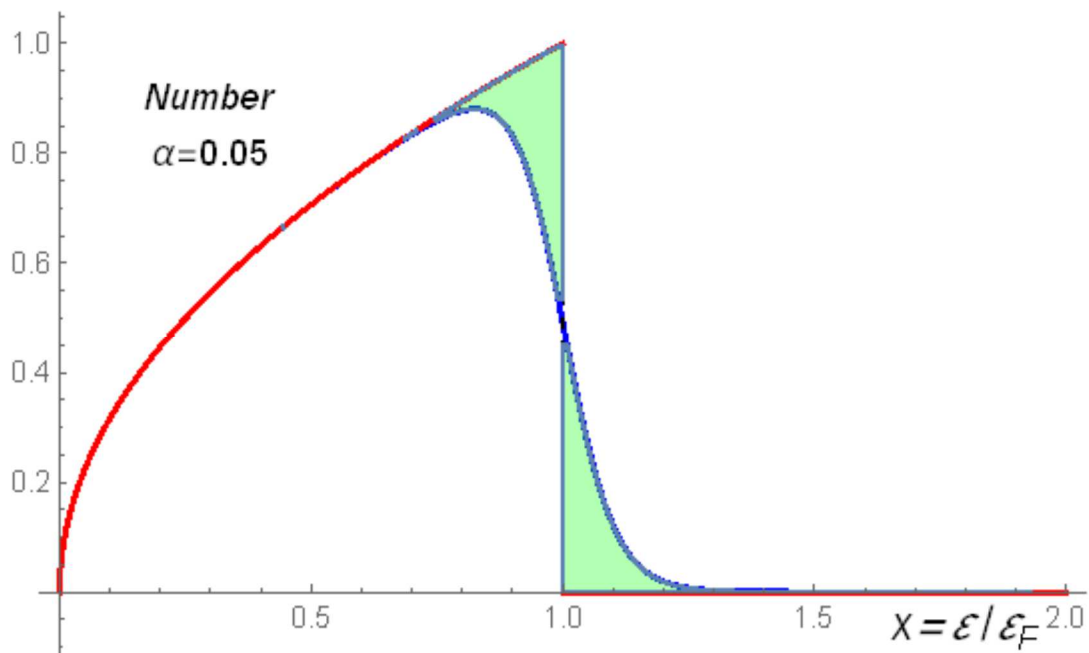
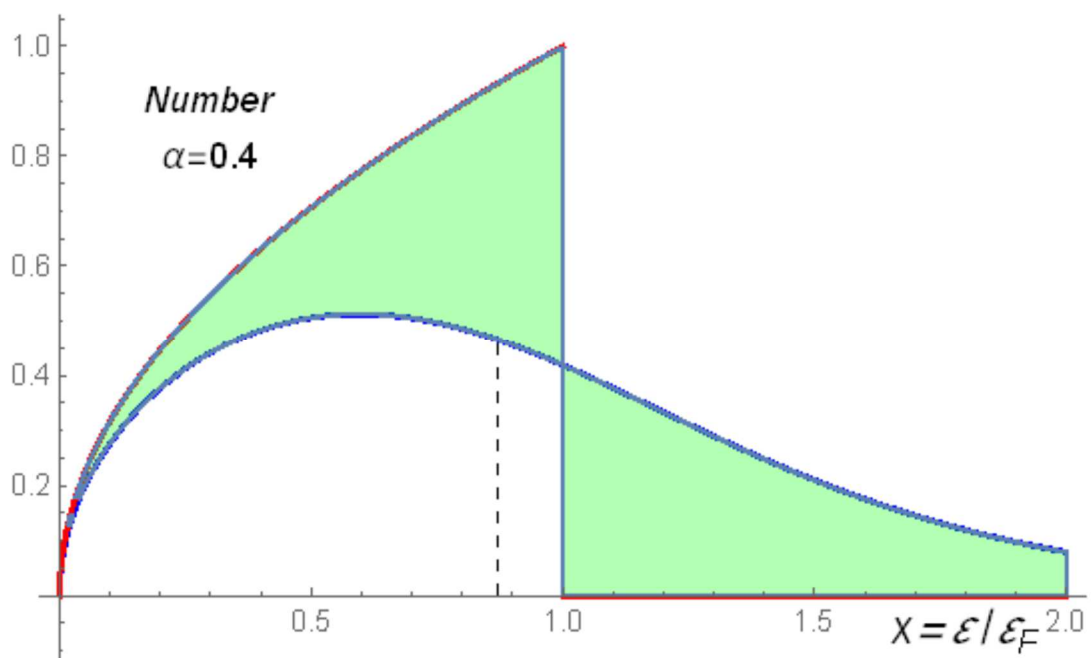
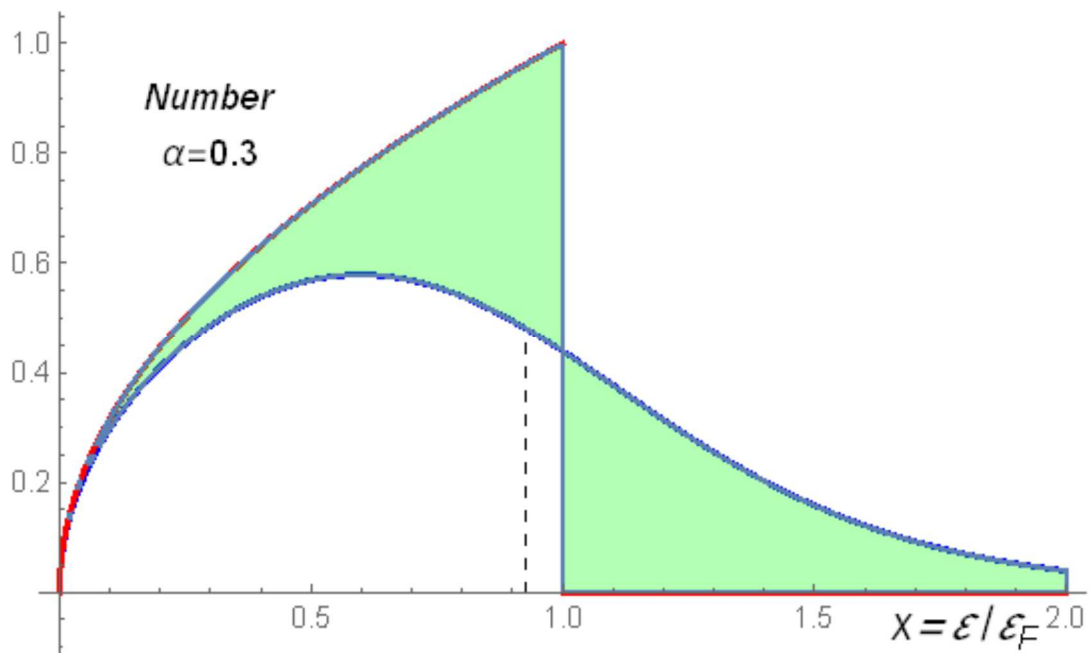


Fig. Chemical potential as a function of temperature for the ideal 3D Fermi gas and the 1D Fermi gas.







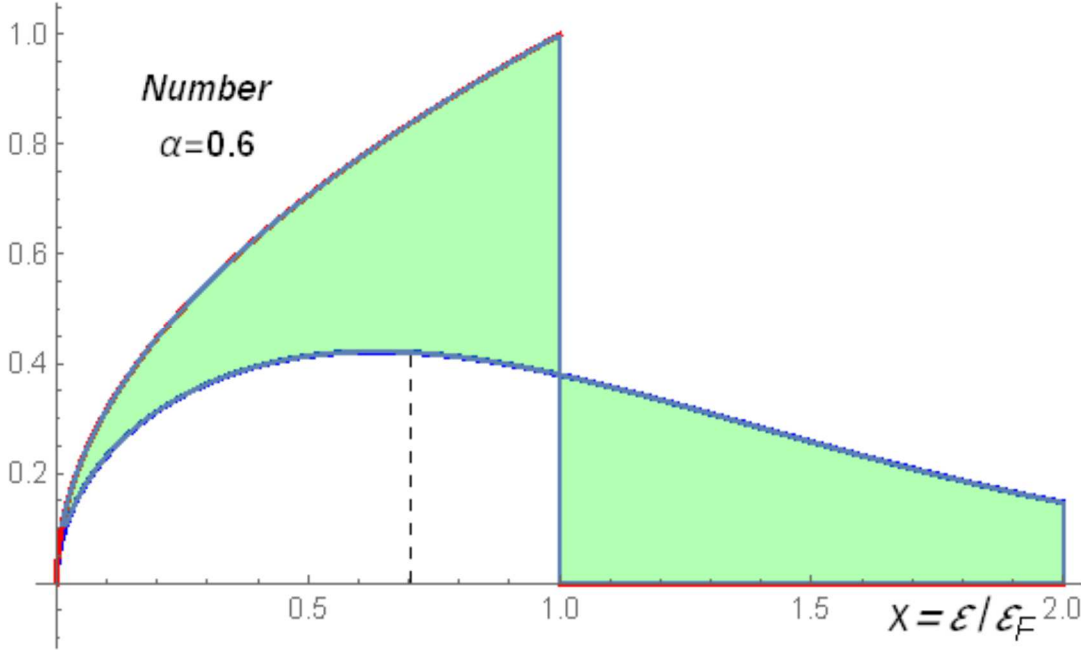


Fig. The number distribution vs $x = \varepsilon / \varepsilon_F$. $\alpha = k_B T / \varepsilon_F = 0.1 - 0.6$ for the 3D case. The chemical potential for the temperature with $\alpha = k_B T / \varepsilon_F$ is denoted by the dashed line. It shifts to the low energy side from the Fermi energy at $T = 0$ K ($x = 1$) with increasing temperature. The area for $x > 1$ (shaded region denoted by green) is the same as the area below $x < 1$.

13. Exact solution for the chemical potential for the 2D case

The density of states for the 2D system is

$$D_2(\varepsilon)d\varepsilon = \frac{2L^2}{(2\pi)^2} 2\pi k dk = \frac{2L^2}{(2\pi)^2} 2\pi \left(\frac{2m}{\hbar^2} \right) \frac{1}{2} d\varepsilon$$

or

$$D_2(\varepsilon)d\varepsilon = \frac{mL^2}{\pi\hbar^2} d\varepsilon, \quad D_2(\varepsilon) = \frac{mL^2}{\pi\hbar^2}$$

The density of states for the 2D system is independent of ε . The chemical potential can be evaluated exactly as follows. In other words, we do not have to use the Sommerfeld approximation.

$$N_{2D} = \int_0^{\varepsilon_F} D_2(\varepsilon)d\varepsilon = \frac{mL^2}{\pi\hbar^2} \varepsilon_F$$

$$N_{2D} = \int_0^{\infty} \frac{D_2(\varepsilon) d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} = \frac{mL^2}{\pi\hbar^2} \int_0^{\infty} \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1}$$

Then we have

$$\varepsilon_F = \frac{\pi\hbar^2}{m} n_{2D}$$

with

$$n_{2D} = \frac{N_{2D}}{L^2}$$

We get

$$\varepsilon_F = \int_0^{\infty} \frac{d\varepsilon}{e^{\beta(\varepsilon-\mu)} + 1} = \int_0^{\infty} \frac{d\varepsilon}{\frac{1}{z} e^{\beta\varepsilon} + 1}$$

We put

$$x = e^{\beta\varepsilon}$$

$$dx = \beta e^{\beta\varepsilon} d\varepsilon = \beta x d\varepsilon$$

$$\begin{aligned} \int_0^{\infty} \frac{d\varepsilon}{\frac{1}{z} e^{\beta\varepsilon} + 1} &= \int_1^{\infty} \frac{dx}{\beta x \left(\frac{1}{z} x + 1 \right)} \\ &= \int_1^{\infty} \frac{z dx}{\beta x (x + z)} \\ &= \frac{1}{\beta} \int_1^{\infty} dx \left(\frac{1}{x} - \frac{1}{x + z} \right) \\ &= \frac{1}{\beta} \left[\ln\left(\frac{x}{x + z}\right) \right]_1^{\infty} \\ &= \frac{1}{\beta} \ln(1 + z) \end{aligned}$$

$$\beta\varepsilon_F = \ln(1 + z)$$

or

$$e^{\beta \varepsilon_F} = 1 + z$$

Thus we have

$$\mu = k_B T \ln(e^{\beta \varepsilon_F} - 1)$$

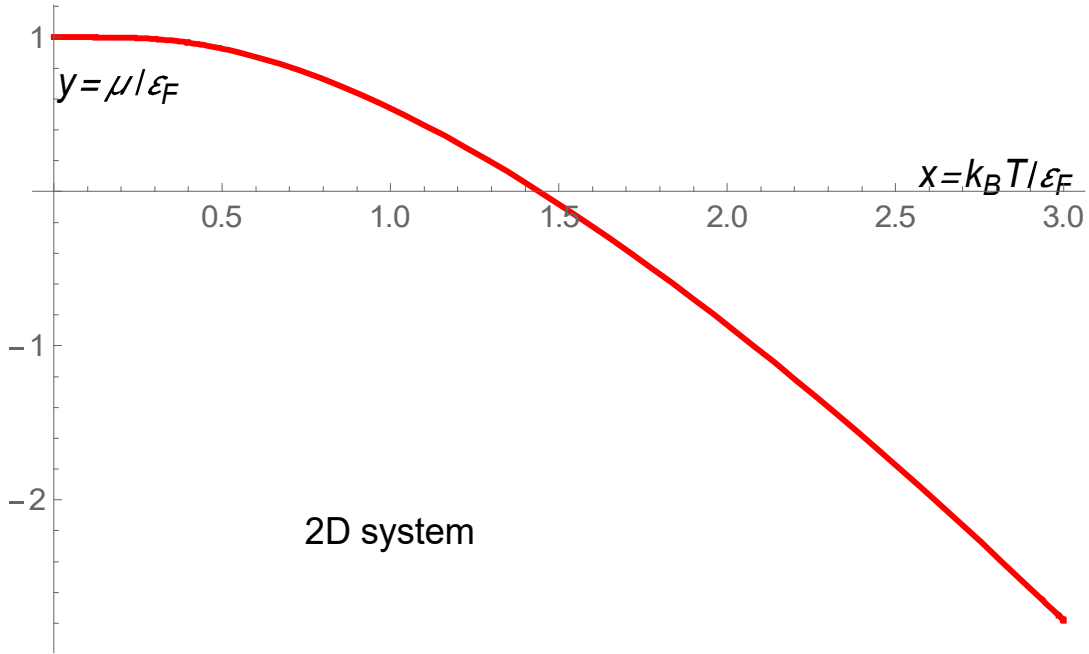


Fig. Chemical potential of the 2D system. Plot of $y = \mu / \varepsilon_F$ as a function of $y = k_B T / \varepsilon_F$

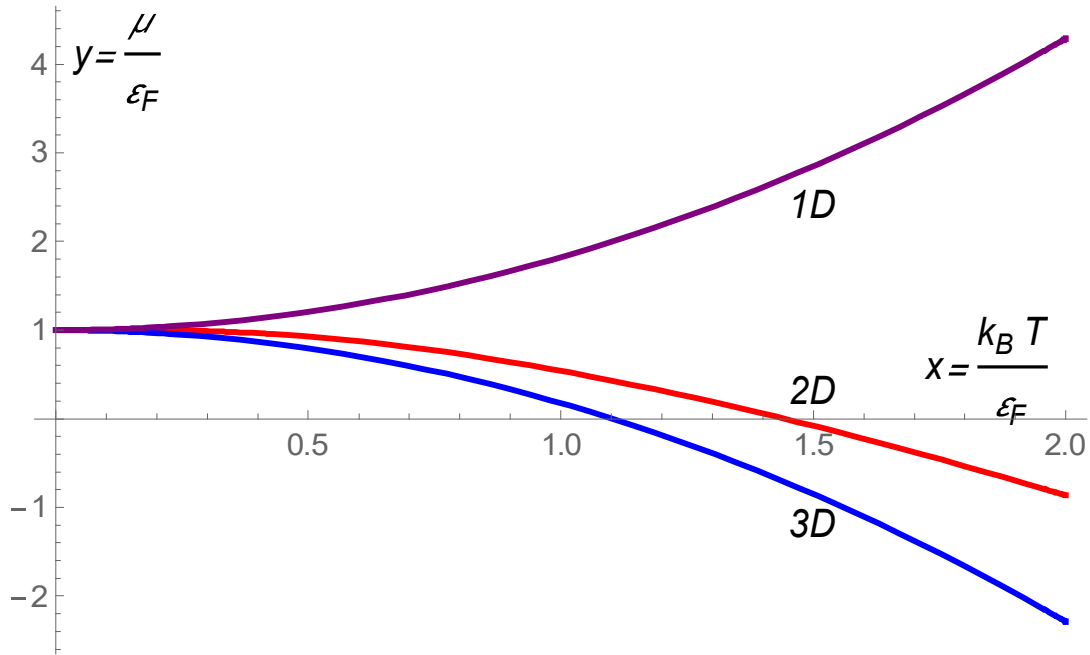


Fig. Chemical potential of the 1D, 2D, and 3D systems. Plot of $y = \mu / \epsilon_F$ as a function of $x = k_B T / \epsilon_F$

REFERENCES

- J. Rau, Statistical Physics and Thermodynamics, An Introduction to Key Concepts (Oxford, 2017).
R. Kubo, Statistical Mechanics An Advanced Course with Problems and Solutions (North-Holland, 1965).
M.D. Sturge, Statistical and Thermal Physics, Fundamentals and Applications (A.K. Peters, 2003).
H.P. Myers, Introductory Solid State Physics, second edition (Taylor and Francis, 1997).