Fermi function

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: November 06, 2017)

We discuss how the chemical potential (the Fermi level) for the 3D, 2D and 1D ideal metals changes with temperature using two methods (equivalent) (i) the method used by Huang (in his textbook) and (ii) the Sommerfeld formula. We make a plot of the Fermi level as a function of temperature. We note that the Fermi energy is the Fermi level at 0 K. The total number and the internal energy of the electrons in metal can be expressed in terms of the Fermi functions. The Fermi function is defined by

$$f_{3/2}(z) = \frac{1}{\Gamma(\frac{3}{2})}\int_0^\infty \frac{y^{1/2}}{e^{y-\nu}+1}dy = \frac{2}{\sqrt{\pi}}\int_0^\infty \frac{y^{1/2}}{e^{y-\nu}+1}dy$$

$$f_{5/2}(z) = \frac{1}{\Gamma(\frac{5}{2})}\int_0^\infty \frac{y^{1/2}}{e^{y-\nu}+1}dy = \frac{4}{3\sqrt{\pi}}\int_0^\infty \frac{y^{3/2}}{e^{y-\nu}+1}dy$$

where $z = e^{\nu}$ and $\nu = \beta\mu$,

$$\Gamma(\frac{1}{2}) = \sqrt{\pi}\,, \qquad \Gamma(\frac{3}{2}) = \frac{\sqrt{\pi}}{2}\,, \qquad \Gamma(\frac{5}{2}) = \frac{3\sqrt{\pi}}{4}$$

1. Total number

The total number is expressed by

$$N = \int_0^\infty \frac{a\sqrt{\varepsilon}}{\frac{1}{z}e^{\beta\varepsilon}+1}d\varepsilon = a\int_0^\infty \frac{\sqrt{\varepsilon}}{\frac{1}{z}e^{\beta\varepsilon}+1}d\varepsilon = ag = a\frac{1}{\beta^{3/2}}\frac{\sqrt{\pi}}{2}f_{3/2}(z)$$

where

$$\nu = \beta\mu\,, \qquad z = e^{\beta\mu} = e^{\nu}\,, \qquad \nu = \ln z\,.$$

We calculate the function defined by

$$g = \int_0^\infty \frac{\sqrt{\varepsilon}}{\frac{1}{z} e^{\beta\varepsilon} + 1} d\varepsilon$$

$$= \frac{1}{\beta^{3/2}} \int_0^\infty \frac{\sqrt{y}}{e^{y-\nu} + 1} dy$$

$$= \frac{1}{\beta^{3/2}} \frac{\sqrt{\pi}}{2} f_{3/2}(z)$$

where

$$y = \beta\varepsilon , \qquad dy = \beta d\varepsilon , \qquad d\varepsilon = \frac{1}{\beta} dy$$

Here the Fermi function is defined as

$$f_{3/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{y}}{e^{y-\nu} + 1} dy$$

(see the references). With a partial integration, this function can be rewritten as

$$f_{3/2}(z) = \frac{4}{3\sqrt{\pi}} \int_0^\infty \frac{y^{3/2} e^{y-\nu}}{(e^{y-\nu} + 1)^2} dy$$

We put $t = y - \nu$; $dy = dt$. Then the function can be rewritten as

$$f_{3/2}(z) \approx \frac{4}{3\sqrt{\pi}} \int_{-\infty}^\infty \frac{(t+\nu)^{3/2} e^t}{(e^t + 1)^2} dt = \frac{2\nu^{3/2}}{3\sqrt{\pi}} \int_{-\infty}^\infty (1 + \frac{t}{\nu})^{3/2} \frac{e^t}{(e^t + 1)^2} dt$$

Note that $f(t) = \dfrac{e^t}{(e^t + 1)^2}$ has a peak at $t = 0$, corresponding to the fact that

$$-\frac{\partial f}{\partial \varepsilon} = \delta(\varepsilon - \varepsilon_F)$$

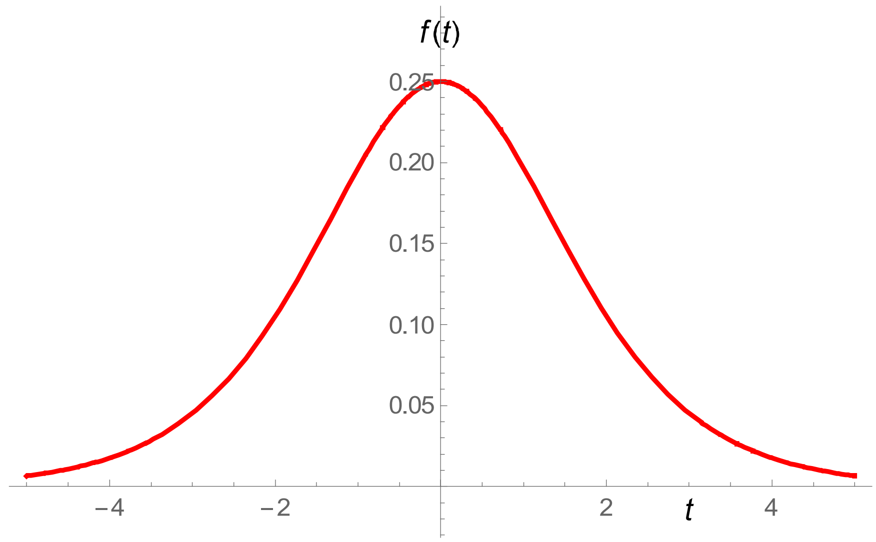

Fig. Function $(t) = \dfrac{e^t}{(e^t+1)^2}$ which has a peak at $t = 0$.

Using the Taylor expansion, we get

$$f_{3/2}(z) = \frac{4\nu^{3/2}}{3\sqrt{\pi}} \int_{-\infty}^{\infty} (1 + \frac{3t^2}{8\nu^2} + \frac{3t^4}{128\nu^4} + \frac{7t^6}{1024\nu^6} + \frac{99t^8}{32768\nu^8} + \frac{429t^{10}}{262144\nu^{10}} + \frac{4199t^{12}}{4194304\nu^{12}} ...)\frac{e^t}{(e^t+1)^2} dt$$

$$= \frac{4\nu^{3/2}}{3\sqrt{\pi}} (I_0 + \frac{3}{8\nu^2} I_2 + \frac{3}{128\nu^4} I_4 + \frac{7}{1024\nu^6} I_6 + \frac{99}{32768\nu^8} I_8$$

$$+ \frac{429}{262144\nu^{10}} I_{10} + \frac{4199}{4194304\nu^{12}} I_{12} + ...)$$

where

$$I_{2n} = 2\int_0^{\infty} \frac{t^{2n} e^t}{(e^t+1)^2} dt \qquad (n;\ \text{positive integer})$$

with

$$I_0 = 1, \qquad I_2 = \frac{\pi^2}{3}, \qquad I_4 = \frac{7\pi^4}{15}, \qquad I_6 = \frac{31\pi^6}{21}, \qquad I_8 = \frac{127\pi^8}{15}$$

$$I_{10} = \frac{2555\pi^{10}}{33}, \qquad I_{12} = \frac{1414477\pi^{12}}{1365}$$

Finally we get the Fermi function as

$$f_{3/2}(z) = \frac{4}{3\sqrt{\pi}}(\nu^{3/2} + \frac{\pi^2}{8\nu^{1/2}} + \frac{3}{128\nu^{5/2}}\frac{7\pi^4}{15} + \frac{7}{1024\nu^{9/2}}\frac{31\pi^6}{21} + \frac{99}{32768\nu^{13/2}}\frac{127\pi^8}{15}$$
$$+ \frac{429}{262144\nu^{17/2}}\frac{2555\pi^{10}}{33} + \frac{4199}{4194304\nu^{21/3}}\frac{1414477\pi^{12}}{1365} + ...)$$

with $\nu = \ln z$

((**Note**))

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

$$N = a\frac{1}{\beta^{3/2}}\frac{\sqrt{\pi}}{2}f_{3/2}(z) = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\frac{1}{\beta^{3/2}}\frac{\sqrt{\pi}}{2}f_{3/2}(z)$$

or

$$\frac{N}{V} = \frac{1}{2}\left(\frac{2mk_BT}{\pi\hbar^2}\right)^{3/2} f_{3/2}(z) = 2n_Q f_{3/2}(z)$$

or

$$\frac{N}{gV}\frac{1}{n_Q} = f_{3/2}(z)$$

where $g = 2$ for spin 1/2 fermion, N corresponds to the total number including spin multiplicity (2). In the classical theory,

$$n = \frac{N}{gV}.$$

2. Fermi level (chemical potential)

The Fermi level (chemical potential) can be derived from

$$N = \int_0^{\varepsilon_F} a\sqrt{\varepsilon}d\varepsilon = \frac{2a}{3}\varepsilon_F{}^{3/2} = a\frac{1}{\beta^{2/3}}\frac{\sqrt{\pi}}{2}f_{3/2}(z)$$

or

$$\frac{4}{3\sqrt{\pi}}(\beta\varepsilon_F)^{3/2} = f_{3/2}(z) = \frac{4}{3\sqrt{\pi}}(\nu^{3/2} + \frac{\pi^2}{8\nu^{1/2}} + \frac{3}{128\nu^{5/2}}\frac{7\pi^4}{15} + \frac{7}{1024\nu^{9/2}}\frac{31\pi^6}{21} + ...)$$

or

$$(\beta\varepsilon_F)^{3/2} = \nu^{3/2} + \frac{\pi^2}{8\nu^{1/2}} + \frac{3}{128\nu^{5/2}}\frac{7\pi^4}{15} + \frac{7}{1024\nu^{9/2}}\frac{31\pi^6}{21} + \frac{99}{32768\nu^{13/2}}\frac{127\pi^8}{15} + \frac{429}{262144\nu^{17/2}}\frac{2555\pi^{10}}{33} + \frac{4199}{4194304\nu^{21/3}}\frac{1414477\pi^{12}}{1365} +$$

with

$$\nu = \beta\mu \qquad \mu(0) = \varepsilon_F$$

In order to find the solution of the chemical potential μ as a function of $\beta\varepsilon_F$, we use the approximation

$$(\beta\varepsilon_F)^{3/2} = \nu^{3/2} + \frac{\pi^2}{8\nu^{1/2}}, \qquad \nu^{3/2} = (\beta\varepsilon_F)^{3/2} - \frac{\pi^2}{8\nu^{1/2}}$$

leading to

$$\begin{aligned}\nu &\approx \beta\varepsilon_F[1 - \frac{\pi^2}{8\nu^{1/2}}(\beta\varepsilon_F)^{-3/2}]^{2/3} \\ &= \beta\varepsilon_F[1 - \frac{\pi^2}{12}(\frac{k_BT}{\varepsilon_F})^2]\end{aligned}$$

or

$$\mu = \varepsilon_F[1 - \frac{\pi^2}{12}(\frac{k_BT}{\varepsilon_F})^2]$$

In other words, the Fermi level decreases with increasing temperature. We evaluate the chemical potential using the Mathematica (ContourPlot) for the several approximations.

$$y = \frac{\mu}{\varepsilon_F}, \qquad x = \frac{k_B T}{\varepsilon_F}$$

(i) $$1 = y^{3/2} + \frac{\pi^2}{8y^{1/2}} x^2$$

(ii) $$1 = y^{3/2} + \frac{\pi^2}{8y^{1/2}} x^2 + \frac{3x^4}{128y^{5/2}} \frac{7\pi^4}{15}$$

(iii)

$$1 = y^{3/2} + \frac{\pi^2}{8y^{1/2}} x^2 + \frac{3x^4}{128y^{5/2}} \frac{7\pi^4}{15} + \frac{7x^6}{1024y^{9/2}} \frac{31\pi^6}{21} + ...$$

(iv)

$$1 = y^{3/2} + \frac{\pi^2}{8y^{1/2}} x^2 + \frac{3x^4}{128y^{5/2}} \frac{7\pi^4}{15} + \frac{7x^6}{1024y^{9/2}} \frac{31\pi^6}{21} + \frac{99x^8}{32768y^{13/2}} \frac{127\pi^8}{15} ...$$

(v)

$$1 = y^{3/2} + \frac{\pi^2}{8y^{1/2}} x^2 + \frac{3x^4}{128y^{5/2}} \frac{7\pi^4}{15} + \frac{7x^6}{1024y^{9/2}} \frac{31\pi^6}{21} + \frac{99x^8}{32768y^{13/2}} \frac{127\pi^8}{15}$$
$$+ \frac{429x^{10}}{262144y^{17/2}} \frac{2555\pi^{10}}{33}$$

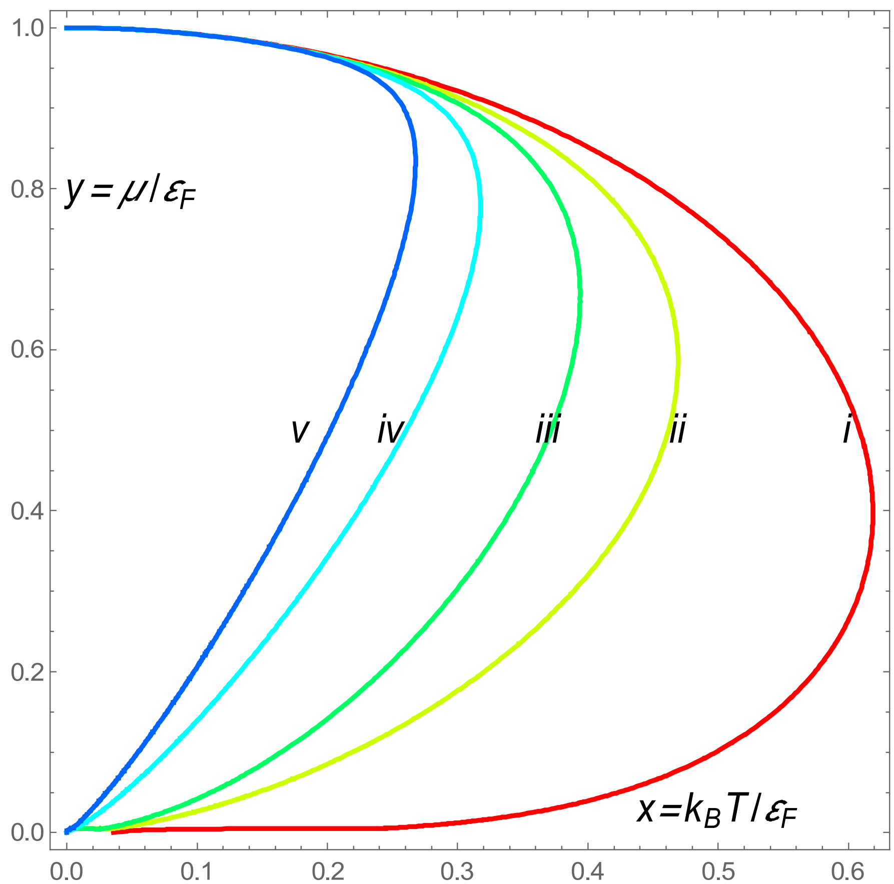

Fig. Plot of $y = \varepsilon / \varepsilon_F$ as a function of $x = k_B T / \varepsilon_F$ for the approximations (i, ii, iii, iv, and v) from the lowest order to the highest order.

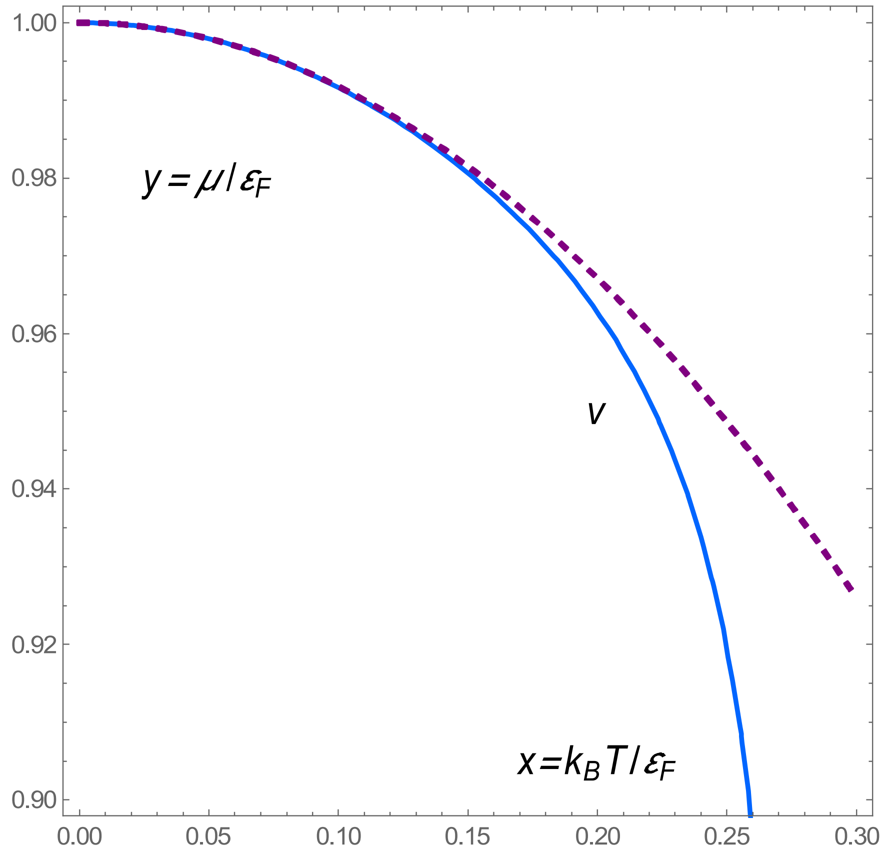

Fig. Plot of $y = \varepsilon / \varepsilon_F$ as a function of $x = k_B T / \varepsilon_F$ for the approximation (v) (denoted by blue) and $y = 1 - \frac{\pi^2}{12} x^2$ (dashed line, purple).

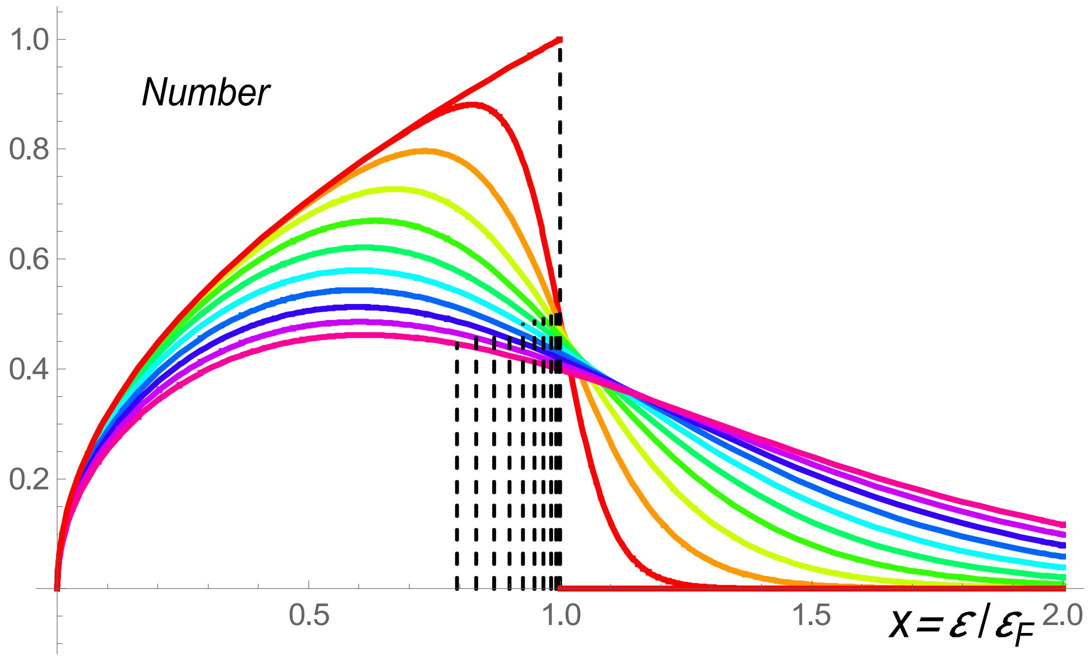

Fig. The number distribution as a function of $x = \varepsilon / \varepsilon_F$. The chemical potential (μ / ε_F) is denoted by dotted line. It decreases with increasing temperature. The parameter $\alpha = k_B T / \varepsilon_F$ is changed as a parameter. $\alpha = 0.05 - 0.5$ with $\Delta\alpha = 0.05$.

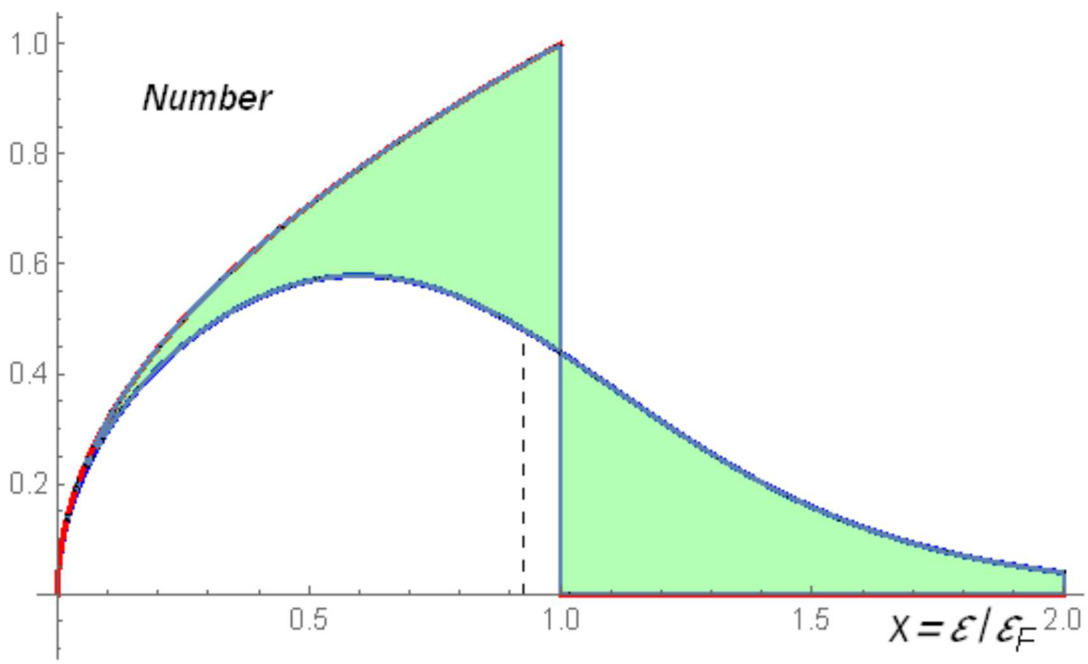

Fig. The number distribution as a function of $x = \varepsilon / \varepsilon_F$. The chemical potential (μ / ε_F) is denoted by dotted line. The parameter $\alpha = k_B T / \varepsilon_F = 0.3$. The shaded region for x<1 is the same as that for x>1.

3. Internal energy U

The internal energy is given by

$$U = \int_0^\infty \frac{a\varepsilon\sqrt{\varepsilon}}{\frac{1}{z}e^{\beta\varepsilon} + 1} d\varepsilon = a\int_0^\infty \frac{\varepsilon^{3/2}}{\frac{1}{z}e^{\beta\varepsilon} + 1} d\varepsilon$$

where

$$\nu = \beta\mu , \qquad z = e^{\beta\mu} = e^{\nu} , \qquad \nu = \ln z .$$

Since $N = \frac{2a}{3}\varepsilon_F^{\ 3/2}$, we get

$$\begin{aligned}
\frac{U}{N} &= \frac{3}{2a}\varepsilon_F^{\ -3/2} a\int_0^\infty \frac{\varepsilon^{3/2}}{\frac{1}{z}e^{\beta\varepsilon} + 1} d\varepsilon \\
&= \frac{3}{2}\varepsilon_F^{\ -3/2} \int_0^\infty \frac{\varepsilon^{3/2}}{\frac{1}{z}e^{\beta\varepsilon} + 1} d\varepsilon \\
&= \frac{3}{2}\varepsilon_F^{\ -3/2} g
\end{aligned}$$

with

$$\begin{aligned}
g &= \int_0^\infty \frac{\varepsilon^{3/2}}{\frac{1}{z}e^{\beta\varepsilon} + 1} d\varepsilon \\
&= \frac{1}{\beta^{5/2}} \int_0^\infty \frac{y^{3/2}}{e^{y-\nu} + 1} dy \\
&= \frac{1}{\beta^{5/2}} \frac{3\sqrt{\pi}}{4} f_{5/2}(z)
\end{aligned}$$

where

$$y = \beta\varepsilon , \qquad dy = \beta d\varepsilon , \qquad d\varepsilon = \frac{1}{\beta} dy$$

Here the Fermi function is defined as

$$f_{5/2}(z) = \frac{4}{3\sqrt{\pi}} \int_0^{\infty} \frac{y^{3/2}}{e^{y-\nu}+1} dy$$

Note that

$$f_{3/2}(z) = z\frac{\partial}{\partial z} f_{5/2}(z) \qquad \text{(see the book of Huang, and Greiner)}$$

With a partial integration, this function can be rewritten as

$$f_{5/2}(z) = \frac{4}{3\sqrt{\pi}} \int_0^{\infty} \frac{y^{3/2}}{e^{y-\nu}+1} dy = \frac{8}{15\sqrt{\pi}} \int_0^{\infty} \frac{y^{5/2}e^{y-\nu}}{(e^{y-\nu}+1)^2} dy .$$

We put $t = y - \nu$; $dy = dt$. Then we have

$$f_{5/2}(z) = \frac{8}{15\sqrt{\pi}} \int_{-\infty}^{\infty} \frac{(t+\nu)^{5/2}e^t}{(e^t+1)^2} dt = \frac{8\nu^{5/2}}{15\sqrt{\pi}} \int_{-\infty}^{\infty} (1+\frac{t}{\nu})^{5/2} \frac{e^t}{(e^t+1)^2} dt$$

using the Taylor expansion, we get

$$\begin{aligned} f_{5/2}(z) &= \frac{8\nu^{5/2}}{15\sqrt{\pi}} \int_{-\infty}^{\infty} (1 + \frac{15t^2}{8\nu^2} - \frac{5t^4}{128\nu^4} - \frac{5t^6}{1024\nu^6} - \frac{45t^8}{32768\nu^8} - \frac{143t^{10}}{262144\nu^{10}} + ...) \frac{e^t}{(e^t+1)^2} dt \\ &= \frac{8\nu^{5/2}}{15\sqrt{\pi}} (I_0 + \frac{15}{8\nu^2} I_2 - \frac{5}{128\nu^4} I_4 - \frac{5}{1024\nu^6} I_6 - \frac{45}{32768\nu^8} I_8 \\ &\quad - \frac{143}{262144\nu^{10}} I_{10} - \frac{1105}{4194304\nu^{12}} I_{12} + ...) \end{aligned}$$

where

$$I_{2n} = 2\int_0^{\infty} \frac{t^{2n}e^t}{(e^t+1)^2} dt$$

with

$$I_0 = 1, \qquad I_2 = \frac{\pi^2}{3}, \qquad I_4 = \frac{7\pi^4}{15}, \qquad I_6 = \frac{31\pi^6}{21}, \qquad I_8 = \frac{127\pi^8}{15}$$

$$\frac{U}{N\varepsilon_F} = \frac{3}{2}\frac{1}{(\beta\varepsilon_F)^{5/2}}\frac{3\sqrt{\pi}}{4}f_{5/2}(z)$$

$$= \frac{3}{5}\frac{\nu^{5/2}}{(\beta\varepsilon_F)^{5/2}}(I_0 + \frac{15}{8\nu^2}I_2 - \frac{5}{128\nu^4}I_4 - \frac{5}{1024\nu^6}I_6 - \frac{45}{32768\nu^8}I_8$$

$$- \frac{143}{262144\nu^{10}}I_{10} - \frac{1105}{4194304\nu^{12}}I_{12} + ...)$$

The first-order approximation;

$$\frac{U}{N\varepsilon_F} = \frac{3}{5}$$

The second-order approximation

$$\frac{U}{N\varepsilon_F} = \frac{3}{5}\left(\frac{\mu}{\varepsilon_F}\right)^{5/2}[1 + \frac{5\pi^2}{8}\left(\frac{\mu}{\varepsilon_F}\right)^{-2}\left(\frac{k_BT}{\varepsilon_F}\right)^2]$$

Using the relation

$$\frac{\mu}{\varepsilon_F} = 1 - \frac{\pi^2}{12}(\frac{k_BT}{\varepsilon_F})^2$$

we have

$$\frac{U}{N\varepsilon_F} \approx \frac{3}{5}[1 - \frac{\pi^2}{12}(\frac{k_BT}{\varepsilon_F})^2]^{5/2}[1 + \frac{5\pi^2}{8}\left(\frac{k_BT}{\varepsilon_F}\right)^2]$$

$$\approx \frac{3}{5}[1 - \frac{5\pi^2}{24}(\frac{k_BT}{\varepsilon_F})^2][1 + \frac{5\pi^2}{8}\left(\frac{k_BT}{\varepsilon_F}\right)^2]$$

$$= \frac{3}{5}[1 + \frac{5\pi^2}{12}(\frac{k_BT}{\varepsilon_F})^2]$$

or

$$U = \frac{3}{5}N\varepsilon_F[1 + \frac{5\pi^2}{12}(\frac{k_BT}{\varepsilon_F})^2]$$

The pressure P:

$$P = \frac{2U}{3V} = \frac{2}{5} n\varepsilon_F [1 + \frac{5\pi^2}{12} (\frac{k_B T}{\varepsilon_F})^2]$$

The heat capacity:

$$\frac{C}{Nk_B} = \frac{1}{2}\pi^2 \frac{k_B T}{\varepsilon_F}.$$

REFERENCES

N.W. Ashcroft and N.D. Mermin, Solid State Physics (Hartcourt, 1976)

K. Huang, Statistical Mechanics (Wiley, 1987).

M. Suzuki and I.S. Suzuki, Free electron Fermi gas model; https://www.binghamton.edu/physics/docs/note-free-electron-gas.pdf

W. Greiner, L. Neise, and H. Stocker, Thermodynamics and Statistical Mechanics (Springer, 1995).