

Condensed Matter Physics (Phy 771)

HW #4 - solution

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① problem 6.1 Marder

The free Fermi gas is described by $H\Psi = E\Psi$ (1)

where $\Psi = \Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N)$ is the total wavefunction of all fermions and

$$H = H_1 + H_2 + \dots + H_i + \dots + H_N = \sum_{i=1}^N H_i = \sum_i \frac{p_i^2}{2m} = \sum_{i=1}^N \frac{-\hbar^2 \nabla_i^2}{2m}$$

where $p_i = -i\hbar \nabla_i$

$$E = E_1 + E_2 + \dots + E_i + \dots + E_N = \sum_i E_i$$

a) let $\Psi(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_N) = \prod_{j=1}^N \psi_j(\vec{r}_j) = \psi_i(\vec{r}_i) \prod_{j \neq i}^N \psi_j(\vec{r}_j)$

now the L.H.S of eqⁿ (1) reads

$$H\Psi = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 \Psi = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 \psi_i(\vec{r}_i) \prod_{j \neq i}^N \psi_j(\vec{r}_j)$$

$$= -\frac{\hbar^2}{2m} \sum_{i=1}^N \prod_{j \neq i}^N \psi_j(\vec{r}_j) \nabla_i^2 \psi_i(\vec{r}_i) ; \frac{-\hbar^2}{2m} \nabla_i^2 \psi_i = E_i \psi_i$$

$$= \sum_{i=1}^N \prod_{j \neq i}^N \psi_j(\vec{r}_j) E_i \psi_i(\vec{r}_i)$$

$$= \sum_{i=1}^N E_i \psi_i(\vec{r}_i) \prod_{j \neq i}^N \psi_j(\vec{r}_j) = \sum_{i=1}^N E_i \prod_{j=1}^N \psi_j(\vec{r}_j) = E\Psi = R.H.S$$

b) similar to part a),

$$\text{let } \psi = \frac{1}{N!} \sum_s (-1)^s \prod_{j=1}^N \psi_{sj}(\vec{r}_j) = \frac{1}{N!} \sum_s (-1)^s \psi_{si}(\vec{r}_i) \prod_{\substack{j=1 \\ j \neq i}}^N \psi_{sj}(\vec{r}_j)$$

so the L.H.S of eqⁿ(1) reads

$$\begin{aligned} H\psi &= -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 \psi = -\frac{\hbar^2}{2m} \sum_{i=1}^N \nabla_i^2 \frac{1}{N!} \sum_s (-1)^s \psi_{si}(\vec{r}_i) \prod_{\substack{j=1 \\ j \neq i}}^N \psi_{sj}(\vec{r}_j) \\ &= \frac{1}{N!} \sum_i \sum_s (-1)^s \prod_{\substack{j=1 \\ j \neq i}}^N \psi_{sj}(\vec{r}_j) \left[\underbrace{-\frac{\hbar^2 \nabla_i^2}{2m} \psi_{si}(\vec{r}_i)}_{\epsilon_i \psi_{si}(\vec{r}_i)} \right] \end{aligned}$$

$$= \frac{1}{N!} \sum_i \sum_s (-1)^s \prod_{\substack{j=1 \\ j \neq i}}^N \psi_{sj}(\vec{r}_j) \epsilon_i \psi_{si}(\vec{r}_i)$$

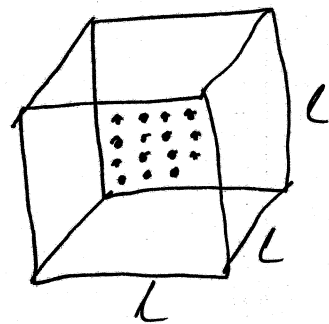
$$= \sum_i \epsilon_i \frac{1}{N!} \sum_s (-1)^s \psi_{si}(\vec{r}_i) \prod_{\substack{j=1 \\ j \neq i}}^N \psi_{sj}(\vec{r}_j)$$

$$= \sum_i \epsilon_i \frac{1}{N!} \sum_s (-1)^s \prod_{j=1}^N \psi_{sj}(\vec{r}_j)$$

$$= \sum_i \epsilon_i \psi = \epsilon \psi = \text{R.H.S} \quad \checkmark$$

② Problem 6.2 Marder:

consider 15 electrons confined in a cube of side length L . Here N is small number, hence we cannot convert sum to integral, instead we will distribute them manually according to



$$E_k = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} (k_x^2 + k_y^2 + k_z^2); \text{ where}$$

$$\vec{k} = (k_x, k_y, k_z)$$

$$= \frac{\hbar^2}{2m} \frac{4\pi^2}{L^2} (n_x^2 + n_y^2 + n_z^2)$$

$$= \frac{2\pi^2 \hbar^2}{mL^2} (n_x^2 + n_y^2 + n_z^2);$$

$$n_x, n_y, n_z = 0, \pm 1, \pm 2, \dots$$

- the lowest energy level $E_0 = 0$ corresponds to $(n_x, n_y, n_z) = (0, 0, 0)$. This state can accept 2 electrons ($\uparrow, \downarrow$) with opposite spins.
- the next energy level $E_1 = \frac{2\hbar^2 \pi^2}{mL^2}$ corresponds to the combinations $(1, 0, 0), (0, 1, 0), (0, 0, 1), (-1, 0, 0), (0, -1, 0), (0, 0, -1)$. This level is 6-fold degenerate and can accept 12 electrons.
- The highest occupied single particle state (level) is $E_2 = \frac{4\hbar^2 \pi^2}{mL^2} = 2E_1$, which corresponds to $(n_x, n_y, n_z) = (1, 1, 0), (1, 0, 1), (0, 1, 1), (-1, 1, 0), (-1, 0, 1), (0, -1, 1), (1, -1, 0), (1, 0, -1), (0, 1, -1), (-1, -1, 0), (-1, 0, -1), (0, -1, -1)$. This level is 12-fold degenerate and can accept 24 electrons. but here we have 1 electron left to this level $\Rightarrow$ the ground state energy is

$$E_2 \quad \underline{1e}$$

$$E_1 \quad \underline{12e}$$

$$E_0 \quad \underline{2e}$$

$$E_{\text{ground state}} = 0 + 12 \left(\frac{2\hbar^2 \pi^2}{mL^2} \right) + \frac{4\hbar^2 \pi^2}{mL^2}$$

$$= 28 \frac{\hbar^2 \pi^2}{mL^2}$$

③ problem 6.3 Marcher:

$$\Omega = -k_B T \int_0^\infty d\varepsilon D(\varepsilon) \ln(1 + e^{\beta(\mu - \varepsilon)})$$

in the zero temperature limit ($T \rightarrow 0$), $\beta \gg 1$, so $e^{\beta(\mu - \varepsilon)} \gg 1$

$$\Rightarrow \ln(1 + e^{\beta(\mu - \varepsilon)}) \approx \ln e^{\beta(\mu - \varepsilon)} = \beta(\mu - \varepsilon) \ln e = \beta(\mu - \varepsilon)$$

furthermore, in the zero temperature limit, $\mu \approx \varepsilon_F$ and

$$D(\varepsilon) = \begin{cases} \kappa V \varepsilon^{1/2}, & \varepsilon < \varepsilon_F \\ 0, & \varepsilon > \varepsilon_F \end{cases}, \text{ so the integral becomes}$$

$$\begin{aligned} \Omega &= -k_B T \int_0^{\varepsilon_F} d\varepsilon \kappa V \varepsilon^{1/2} \beta(\varepsilon_F - \varepsilon) = -\kappa V \int_0^{\varepsilon_F} d\varepsilon \varepsilon^{1/2} (\varepsilon_F - \varepsilon) \\ &= -\kappa V \left[\varepsilon_F \int_0^{\varepsilon_F} \varepsilon^{1/2} d\varepsilon - \int_0^{\varepsilon_F} \varepsilon^{3/2} d\varepsilon \right] = -\kappa V \left[\frac{2}{3} \varepsilon_F^{5/2} - \frac{2}{5} \varepsilon_F^{5/2} \right] \end{aligned}$$

$$= -\frac{4}{15} \kappa V \varepsilon_F^{5/2}$$

$$\text{now } P = -\left(\frac{\partial \Omega}{\partial V}\right)_{T, \mu} = \frac{4}{15} \kappa \varepsilon_F^{5/2}$$

$$= \frac{2}{5} \left(\frac{2}{3} \kappa \varepsilon_F^{3/2} \right) \varepsilon_F; \text{ but } N = \frac{2}{3} \kappa V \varepsilon_F^{3/2} \Rightarrow \frac{N}{V} = n = \frac{2}{3} \kappa \varepsilon_F^{3/2}$$

$$= \frac{2}{5} n \varepsilon_F; \text{ for copper and using table 6.1 } n = 8.49 \times 10^{28} / \text{m}^3, \varepsilon_F = 7.04 \text{ eV}$$

$$\Rightarrow P_{\text{Cu}} = \frac{2}{5} (8.49 \times 10^{28}) (7.04 \times 1.6 \times 10^{-19}) = 3.8 \times 10^{10} \text{ J/m}^3 = 3.8 \times 10^{10} \text{ Pa}$$

$$= \frac{3.8 \times 10^{10} \text{ Pa}}{1.013 \times 10^5 \text{ Pa/atm}} = 3.7 \times 10^5 \text{ atm} !!$$

huge pressure for electrons
gas in Cu at
 $T = 300 \text{ K}$

④ problem 6.4 Marder (modified)

a) Electron gas in 2D ($d=2$)

$$D(\epsilon) = \frac{2}{(2\pi)^2} \int d^2q d^2k \delta(\epsilon - \epsilon_q) ; \quad \epsilon_q = \frac{\hbar^2 k^2}{2m}$$

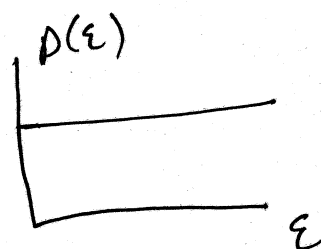
$$= \frac{2}{(2\pi)^2} \underbrace{\int d^2q}_A \int k dk d\phi \delta(\epsilon - \epsilon_q) ; \quad \begin{array}{l} 0 \leq k < k_F \\ 0 < \phi < 2\pi \end{array}$$

$$= \frac{4\pi A}{4\pi^2} \int_0^\infty dk k \delta(\epsilon - \epsilon_q)$$

; where $d^2k = k dk d\phi$
in polar coordinates
; and $k^2 = \frac{2m}{\hbar^2} \epsilon_q$
 $k dk = \frac{m}{\hbar^2} d\epsilon_q$

$$= \frac{A m}{\pi \hbar^2} \underbrace{\int_0^\infty d\epsilon_q \delta(\epsilon - \epsilon_q)}_1 = \frac{A m}{\pi \hbar^2}$$

$$= \text{constant} \quad \text{where } \kappa = A/\pi \hbar^2$$



- now from $N = \int_0^{\epsilon_F} d\epsilon D(\epsilon) f(\epsilon) ; f(\epsilon) = 1$

$$\Rightarrow N = \kappa A \int_0^{\epsilon_F} d\epsilon = \kappa A \epsilon_F \Rightarrow \epsilon_F = \frac{1}{\kappa} \underbrace{\left(\frac{N}{A} \right)}_n = \frac{\pi \hbar^2 n}{m} \checkmark$$

$$\text{and } E = \int_0^{\epsilon_F} d\epsilon \epsilon D(\epsilon) f(\epsilon) = \kappa A \int_0^{\epsilon_F} \epsilon d\epsilon = \kappa A \frac{\epsilon_F^2}{2} = \frac{A m}{\pi \hbar^2} \frac{\epsilon_F^2}{2}$$

$$= \frac{A m}{2\pi \hbar^2} \epsilon_F \epsilon_F = \frac{A m}{2\pi \hbar^2} \cdot \frac{n \pi \hbar^2}{m} \epsilon_F = \frac{1}{2} A n \epsilon_F = \frac{1}{2} A \frac{N}{A} \epsilon_F$$

$$= \frac{1}{2} N \epsilon_F \Rightarrow \boxed{\frac{E}{N} = \frac{1}{2} \epsilon_F} \checkmark$$

- equation of state reads $P A = \frac{2}{3} E \Rightarrow P = \frac{2}{3} \frac{E}{A}$

$$\Rightarrow P = \frac{2}{3} \cdot \frac{\frac{1}{2} A n \epsilon_F}{A} = \frac{1}{3} n \epsilon_F$$

b) Electron gas in 1D ($d=1$)

$$D(\epsilon) = \underbrace{\frac{2}{(2\pi)}}_{\text{from spin}} \cdot 2 \cdot \int dk \delta(\epsilon - \epsilon_p) ; \quad \epsilon_p = \frac{\hbar^2 k^2}{2m} \text{ as before}$$

This factor comes from the fact that in 1D, k can take both positive and negative values

$$\Rightarrow k^2 = \frac{2m}{\hbar^2} \epsilon_p$$

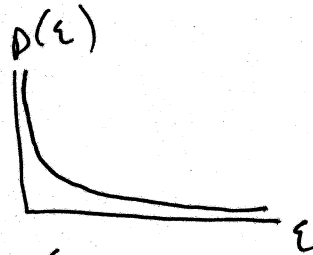
$$k = \left(\frac{2m}{\hbar^2}\right)^{1/2} \epsilon_p^{1/2}$$

$$dk = \frac{(2m)^{1/2}}{\hbar} \cdot \frac{1}{2} \epsilon_p^{-1/2} d\epsilon_p$$

(two-fold degenerate) in comparison with 2D and 3D cases, where k is always positive, so

$$\Rightarrow D(\epsilon) = \frac{2}{\pi} \int_0^L dk \delta(\epsilon - \epsilon_p) = \frac{2L}{\pi} \frac{(2m)^{1/2}}{2\hbar} \underbrace{\int_0^\infty \epsilon_p^{-1/2} d\epsilon_p \delta(\epsilon - \epsilon_p)}_{\epsilon^{-1/2}}$$

$$= \frac{L}{\pi\hbar} \sqrt{\frac{2m}{\epsilon}} \Rightarrow$$



$$\Rightarrow N = \int_0^{\epsilon_F} d\epsilon D(\epsilon) f(\epsilon) = \frac{L}{\pi\hbar} \sqrt{2m} \int_0^{\epsilon_F} \epsilon^{-1/2} d\epsilon = \frac{2L}{\pi\hbar} \sqrt{2m} \epsilon_F^{1/2}$$

$$\Rightarrow \frac{N}{L} = n = \frac{2}{\pi\hbar} \sqrt{2m} \epsilon_F^{1/2} \Rightarrow \epsilon_F = \frac{n^2 \pi^2 \hbar^2}{8m} ; f(\epsilon) = 1$$

$$\text{and } E = \int_0^{\epsilon_F} d\epsilon D(\epsilon) \epsilon f(\epsilon) = \frac{L}{\pi\hbar} \sqrt{2m} \int_0^{\epsilon_F} \epsilon^{1/2} d\epsilon = \frac{2}{3} \frac{L}{\pi\hbar} \sqrt{2m} \epsilon_F^{3/2}$$

$$= \frac{L}{3} \underbrace{\frac{2}{\pi\hbar} \sqrt{2m} \epsilon_F^{1/2}}_{N/L} \epsilon_F = \frac{1}{3} N \epsilon_F \Rightarrow \boxed{\frac{E}{N} = \frac{1}{3} \epsilon_F}$$

- equation of state reads $PL = \frac{2}{3} E \Rightarrow P = \frac{2}{3} \frac{E}{L}$

$$\Rightarrow P = \frac{2}{3} \cdot \frac{1}{3} n \epsilon_F = \frac{2}{9} n \epsilon_F = \frac{1}{3} n \epsilon_F \Rightarrow P = \begin{cases} \frac{2}{5} n \epsilon_F, & 3D \\ \frac{1}{3} n \epsilon_F, & 2D, 1D \end{cases}$$

⑤ Problem 6.8 Marder

a) $N = \kappa V \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{e^{\beta(\epsilon - \mu)} + 1}$; where $\kappa = \frac{(2m)^{3/2}}{2\pi^2 \hbar^3} = 1.062 \times 10^{56} \frac{m^{-3}}{J^{-3/2}}$

$$\frac{N}{V} = n = \kappa \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{e^{\beta(\epsilon - \mu)} + 1}$$

$m = 9.11 \times 10^{-31} \text{ kg}$
 $\hbar = 1.054 \times 10^{-34} \text{ J.s}$

$\Rightarrow \frac{n}{\kappa} = \int_0^\infty \frac{\epsilon^{1/2} d\epsilon}{e^{\beta(\epsilon - \mu)} + 1}$, let $\beta\epsilon = x \Rightarrow \epsilon = \frac{x}{\beta}$, $d\epsilon = \frac{dx}{\beta}$

$\Rightarrow \frac{n}{\kappa} = \frac{1}{\beta^{3/2}} \int_0^\infty \frac{x^{1/2} dx}{e^{(x - \beta\mu)} + 1} \Rightarrow \frac{n \beta^{3/2}}{\kappa} = \int_0^\infty \frac{x^{1/2} dx}{e^{(x - \beta\mu)} + 1}$

$\Rightarrow \frac{n}{\kappa (k_B T)^{3/2}} = \int_0^\infty \frac{x^{1/2} dx}{e^{(x - \beta\mu)} + 1}$

for Aluminum (Al), $n = 18.1 \times 10^{28} / m^3$ (table 6.1) $\Rightarrow$

and $k_B = 1.38 \times 10^{-23} \text{ J/K} \Rightarrow$

$\frac{n}{\kappa (k_B)^{3/2}} \frac{1}{T^{3/2}} = \int_0^\infty \frac{x^{1/2} dx}{e^{(x - \beta\mu)} + 1}$

$\frac{18.1 \times 10^{28}}{1.062 \times 10^{56} \times (1.38 \times 10^{-23})^{3/2}} \frac{1}{T^{3/2}} = \int_0^\infty \frac{\sqrt{x} dx}{e^{(x - \beta\mu)} + 1}$

$\frac{3.32 \times 10^7}{T^{3/2}} = \int_0^\infty \frac{\sqrt{x} dx}{e^{(x - \beta\mu)} + 1} \dots \dots (1)$

in Kelvin

The last integral equation can be solved numerically for ($T > 0$ K) to find the roots ($\beta\mu$) and hence the chemical potential μ . At $T=0$ K, $\mu = \varepsilon_F = \underline{11.668 \text{ eV}}$ for Aluminum (see table 6.1)

To find the roots of the integral, use the online WolframAlpha (<https://www.wolframalpha.com/>) as shown below

- i) $T=300$ K, The L.H.S of equation (1) reads 6392 and letting $b = \beta\mu$, we obtain



FindRoot[NIntegrate[Sqrt(x)/(Exp[x-b]+1), {x, 0, Infinity}]==6392, {b,1}]

NATURAL LANGUAGE MATH INPUT EXTENDED KEYBOARD EXAMPLES UPLOAD RANDOM

An attempt was made to fix mismatched parentheses, brackets, or braces.

Input

FindRoot[NIntegrate[$\frac{\sqrt{x}}{\exp(x-b)+1}$, {x, 0, ∞ }] = 6392, {b, 1}]

Result

{b -> 450.589}

initial value

$\Rightarrow \beta\mu = 450.589 \Rightarrow \frac{\mu}{k_B T} = 450.589$

$$\Rightarrow \mu = (k_B T) (450.589) = (8.617 \times 10^{-5} \frac{\text{eV}}{\text{K}} \times 300 \text{ K}) (450.589) = \underline{11.648 \text{ eV}}$$

- ii) $T=10,000$ K, The L.H.S of equation (1) reads 33.21 and letting $b = \beta\mu$, we obtain



FindRoot[NIntegrate[Sqrt(x)/(Exp[x-b]+1), {x, 0, Infinity}]==33.21, {b,1}]

NATURAL LANGUAGE MATH INPUT EXTENDED KEYBOARD EXAMPLES UPLOAD RANDOM

An attempt was made to fix mismatched parentheses, brackets, or braces.

Input

FindRoot[NIntegrate[$\frac{\sqrt{x}}{\exp(x-b)+1}$, {x, 0, ∞ }] = 33.21, {b, 1}]

Result

{b -> 13.4773}

$$\mu = (k_B T) (13.4773) = (8.617 \times 10^{-5} \times 10000) (13.4773) = \underline{11.613 \text{ eV}}$$

b) μ can also be calculated using sommerfeld expansion formula

$$\mu(T) = \epsilon_F - \frac{\pi^2}{12} \frac{(k_B T)^2}{\epsilon_F} ; \quad \epsilon_F = 11.668 \text{ eV}$$

- at 300 K $\Rightarrow k_B T = 0.026 \text{ eV}$

$$\Rightarrow \mu(300 \text{ K}) = 11.668 - 4.7 \times 10^{-5} \approx 11.668 \text{ same as } \mu(T=0 \text{ K})$$

- at 10,000 K $\Rightarrow (k_B T) = 0.862 \text{ eV}$

$$\Rightarrow \mu(10,000 \text{ K}) = 11.668 - 0.052 = 11.616 \text{ eV}$$

c) $f(\epsilon) = \frac{1}{e^{\beta\epsilon - \beta\mu} + 1} ; \text{ at } 300 \text{ K}, f(\epsilon) = \frac{1}{e^{\frac{\epsilon}{0.026} - 450.589} + 1}$

and at 10,000 K, $f(\epsilon) = \frac{1}{e^{\frac{\epsilon}{0.862} - 13.477} + 1}$

 WolframAlpha

Plot [(1/(Exp (x/0.026-450.589)+1), 1/(Exp (x/0.862-13.4773)+1)), {x,0,20}]

NATURAL LANGUAGE

MATH INPUT

EXTENDED KEYBOARD

EXAMPLES

UPLOAD

RANDOM

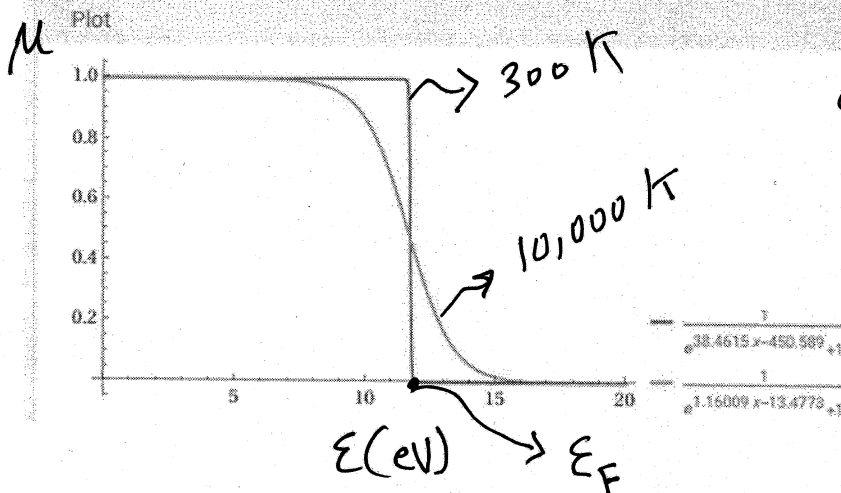
Input interpretation

plot

$$\frac{1}{\exp\left(\frac{x}{0.026} - 450.589\right) + 1}$$

x = 0 to 20

$$\frac{1}{\exp\left(\frac{x}{0.862} - 13.4773\right) + 1}$$



⑥ for 2D electron gas, we found in problem 6.4 that

$$D(\epsilon) = \frac{Am}{\pi \hbar^2} \quad \text{and} \quad \epsilon_F = \frac{\pi \hbar^2 N}{mA} \Rightarrow D(\epsilon) = \frac{N}{\epsilon_F}, \text{ so}$$

$$N = \int_0^\infty d\epsilon D(\epsilon) f(\epsilon) = \frac{N}{\epsilon_F} \int_0^\infty \frac{d\epsilon}{e^{\beta(\epsilon-\mu)} + 1}$$

$$\Rightarrow \epsilon_F = \int_0^\infty \frac{d\epsilon}{e^{\beta(\epsilon-\mu)} + 1} = \int_0^\infty \frac{d\epsilon e^{-\beta(\epsilon-\mu)}}{1 + e^{-\beta(\epsilon-\mu)}} = -\frac{1}{\beta} \int_0^\infty \frac{-\beta e^{-\beta(\epsilon-\mu)} d\epsilon}{1 + e^{-\beta(\epsilon-\mu)}}$$

$$= -k_B T \ln [1 + e^{-\beta(\epsilon-\mu)}] \Big|_0^\infty = -k_B T [0 - \ln(1 + e^{\beta\mu})]$$

$$\epsilon_F = k_B T \ln(1 + e^{\beta\mu}) \Rightarrow \frac{\epsilon_F}{k_B T} = \ln(1 + e^{\beta\mu})$$

$$\Rightarrow e^{\epsilon_F/k_B T} = 1 + e^{\beta\mu} \Rightarrow e^{\beta\mu} = e^{\epsilon_F/k_B T} - 1$$

$$\Rightarrow \beta\mu = \ln[e^{\epsilon_F/k_B T} - 1] \Rightarrow \boxed{\mu = k_B T \ln[e^{\epsilon_F/k_B T} - 1]}$$

- low T limit ($k_B T \ll \epsilon_F$) $\Rightarrow e^{\epsilon_F/k_B T} \gg 1$

$$\Rightarrow \mu = k_B T \frac{\epsilon_F}{k_B T} = \epsilon_F$$

- high T limit ($k_B T \gg \epsilon_F$):

where I used $e^x \approx 1 + x$ for $x \ll 1$

$$\Rightarrow \mu = k_B T \ln \left[1 + \frac{\epsilon_F}{k_B T} - 1 \right]$$

$$= k_B T \ln \frac{\epsilon_F}{k_B T}$$

note that $\mu = 0$ when $\ln \frac{\epsilon_F}{k_B T} = 0 \Rightarrow \frac{\epsilon_F}{k_B T} = 1 \Rightarrow T = T_F = \frac{\epsilon_F}{k_B}$

