Homework 2

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1. Using the second quantized formalism, show that for noninteracting fermions

$$\Omega_0 = -k_B T \sum_i \ln\left[1 + e^{-\beta(\varepsilon_i - \mu)}\right],$$

where ε_i denotes the i-th one-particle level

Solution. The second quantized form of $\hat{K}_0$ is

$$\begin{aligned}
\hat{K}_0 &= \int \mathrm{d}x \hat{\Psi}^\dagger(x) \left[-\frac{\hbar^2}{2M}\triangle + U(x) - \mu\right] \hat{\Psi}(x) \\
&= \sum_{l,m} \int \mathrm{d}x \varphi_k^*(x) \underbrace{\left[-\frac{\hbar^2}{2M}\triangle + U(x) - \mu\right] \varphi_m(x)}_{(\varepsilon_m - \mu)\varphi_m(x)} \hat{a}_l^\dagger \hat{a}_m \\
&= \sum_{l,m} (\varepsilon_m - \mu)\delta_{lm} \hat{a}_l^\dagger \hat{a}_m \\
&= \sum_l (\varepsilon_l - \mu)\hat{a}_l^\dagger \hat{a}_l = \sum_l (\varepsilon_l - \mu)\hat{n}_l
\end{aligned}$$

Using this result,

$$\begin{aligned}
\Omega_0 &= -k_B T \ln Z_G \\
&= -k_B T \ln \mathrm{Tr}\left[e^{-\beta \hat{K}_0}\right] \\
&= -k_B T \ln \mathrm{Tr}\left[e^{-\beta(\hat{H}_0 - \mu\hat{N})}\right] \\
&= -k_B T \ln \mathrm{Tr}\left[e^{-\beta \sum\limits_l (\varepsilon_l - \mu)\hat{a}_l^\dagger \hat{a}_l}\right] \\
&= -k_B T \ln \sum_{\{n_i\}} \left\langle n_1, \ldots, n_i, \ldots \middle| e^{-\beta \sum\limits_l (\varepsilon_l - \mu)\hat{a}_l^\dagger \hat{a}_l} \middle| n_1, \ldots, n_i, \ldots \right\rangle \\
&= -k_B T \ln \sum_{\{n_i\}} e^{-\beta \sum\limits_l (\varepsilon_l - \mu) n_l} \langle n_1, \ldots, n_i, \ldots | n_1, \ldots, n_i, \ldots \rangle \\
&= -k_B T \ln \sum_{\{n_i\}} \prod_{l=1}^{\infty} e^{-\beta(\varepsilon_l - \mu) n_l} = -k_B T \ln \sum_{n_1=0}^{1} \sum_{n_2=0}^{1} \cdots \prod_{l=1}^{\infty} e^{-\beta(\varepsilon_l - \mu) n_l} \\
&= -k_B T \ln \prod_{l=1}^{\infty} \sum_{n_l=0}^{1} e^{-\beta(\varepsilon_l - \mu) n_l} = -k_B T \ln \prod_{l=1}^{\infty} \left(1 + e^{-\beta(\varepsilon_l - \mu)}\right) \\
&= -k_B T \sum_{l=1}^{\infty} \ln\left[1 + e^{-\beta(\varepsilon_l - \mu)}\right]
\end{aligned}$$

Bonus: for bosons, we have

$$\begin{aligned}
\Omega_0 &= -k_B T \ln \prod_{l=1}^{\infty} \sum_{n_l=0}^{\infty} e^{-\beta(\varepsilon_l - \mu) n_l} \\
&= -k_B T \ln \prod_{l=1}^{\infty} \frac{1}{1 - e^{-\beta(\varepsilon_l - \mu)}} \\
&= +k_B T \sum_{l=1}^{\infty} \ln\left[1 - e^{-\beta(\varepsilon_l - \mu)}\right]
\end{aligned}$$

2. Using the result for Ω_0, calculate Ω_0 and N as a function of (T, V, μ) for a fermionic homogeneous system (noninteracting fermions in a box with periodic boundary conditions). Express your result with Fermi-Dirac integrals. Give the first three terms of the high temperature expansion for Ω_0 and for N.

   Solution. For a homogeneous fermionic system, we have

$$\sum_l \longrightarrow \sum_s \frac{V}{(2\pi)^3} \int \mathrm{d}^3\mathbf{k} = (2S+1)\frac{V}{2\pi^2} \int_0^\infty \mathrm{d}k k^2$$

$$\varepsilon_l \longrightarrow \varepsilon(\mathbf{k}, s) = \frac{\hbar^2 k^2}{2m}$$

   Using these, we have

$$\Omega_0 = -k_B T (2S+1) \frac{V}{2\pi^2} \int_0^\infty \mathrm{d}k k^2 \ln\left[1 + e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}\right]$$

   We apply integration by parts:

$$\Omega_0 = -k_B T (2S+1) \frac{V}{2\pi^2} \left[\underbrace{\left[\ln\left(1 + e^{-\beta\ldots}\right) \frac{k^3}{3}\right]_0^\infty}_{=\ln 1 \cdot \infty - 0 \cdot \ln 2 = 0} - \int_0^\infty \mathrm{d}k \frac{k^3}{3} \frac{\partial}{\partial k} \ln\left[1 + \ldots\right] \right]$$

$$\frac{\partial}{\partial k} \ln\left[1 + e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}\right] = \frac{e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}}{1 + e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}} \left(\frac{-\beta\hbar^2}{m}\right) k$$

$$\begin{aligned}
\implies \Omega_0 &= -k_B T (2S+1) \frac{V}{2\pi^2} \int_0^\infty \mathrm{d}k k^4 \frac{\beta\hbar^2}{3m} \frac{e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}}{1 + e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}} \\
&= -k_B T (2S+1) \frac{V\beta\hbar^2}{6\pi^2 m} \int_0^\infty \mathrm{d}k \frac{k^4}{e^{+\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)} + 1}.
\end{aligned}$$

   In order to be able to get to the Dirac integrals, we have to use the following substitutions:

$$x = \frac{\beta\hbar^2 k^2}{2m} \implies k = \left(\frac{2m}{\beta\hbar^2}\right)^{1/2} x^{1/2} \implies \mathrm{d}k = \frac{1}{2}\left(\frac{2m}{\beta\hbar^2}\right)^{1/2} x^{-1/2} \mathrm{d}x$$

$$\alpha = -\beta\mu$$

   With these substitutions,

$$\Omega_0 = -k_B T (2S+1) \frac{V\beta\hbar^2}{6\pi^2 m} \frac{1}{2} \left(\frac{2m}{\beta\hbar^2}\right)^{5/2} \int_0^\infty \mathrm{d}x \frac{x^{3/2}}{e^{x+\alpha} + 1}$$

   The complete Fermi-Dirac integral is defined as

$$F_j(\alpha) = \frac{1}{\Gamma(j+1)} \int_0^\infty \mathrm{d}x \frac{x^j}{e^{x-\alpha} + 1}$$

3. For noninteracting fermions, one can define a characteristic temperature T_{deg} by which the chemical potential is zero:

$$\mu(T = T_{\text{deg}}) = 0.$$

By dimensional analysis

$$k_B T_{\text{deg}} = z \frac{\hbar^2}{2m} \left(\frac{N}{V} \right)^{2/3},$$

where z is a dimensionless number. Calculate z exactly and numerically.

4. Let us suppose that we have N noninteracting, spinless bosons confined in a 3 dimensional harmonic oscillator potential

$$V(\mathbf{r}) = \frac{m}{2}(\omega_1^2 x^2 + \omega_2^2 y^2 + \omega_3^2 z^2).$$

Calculate T_c, where Bose-Einstein condensation occurs.