Statistical physics cheat sheet

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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

$$\hat{K}_{0} = \int dx \hat{\Psi}^{\dagger}(x) \left[-\frac{\hbar^{2}}{2M} \triangle + U(x) - \mu \right] \hat{\Psi}(x)$$

$$= \sum_{l,m} \int dx \varphi_{k}^{*}(x) \underbrace{\left[-\frac{\hbar^{2}}{2M} \triangle + U(x) - \mu \right] \varphi_{m}(x)}_{(\varepsilon_{m} - \mu)\varphi_{m}(x)} \hat{a}_{l}^{\dagger} \hat{a}_{m}$$

$$= \sum_{l,m} (\varepsilon_{m} - \mu) \delta_{lm} \hat{a}_{l}^{\dagger} \hat{a}_{m}$$

$$= \sum_{l} (\varepsilon_{l} - \mu) \hat{a}_{l}^{\dagger} \hat{a}_{l} = \sum_{l} (\varepsilon_{l} - \mu) \hat{n}_{l}$$

Using this result,

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

Bonus: for bosons, we have

$$\Omega_0 = -k_B T \ln \prod_{l=1}^{\infty} \sum_{n_l=0}^{\infty} e^{-\beta(\varepsilon_l - \mu)n_l}$$

$$= -k_B T \ln \prod_{l=1}^{\infty} \frac{1}{1 - e^{-\beta(\varepsilon_l - \mu)}}$$

$$= +k_B T \sum_{l=1}^{\infty} \ln \left[1 - e^{-\beta(\varepsilon_l - \mu)}\right]$$

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

$$\sum_{l} \longrightarrow \sum_{s} \frac{V}{(2\pi)^{3}} \int d^{3}\mathbf{k} = (2S+1) \frac{V}{2\pi^{2}} \int_{0}^{\infty} dk k^{2}$$

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

Using these, we have

$$\Omega_0 = (2S+1)\frac{V}{2\pi^2} \int_{0}^{\infty} dk k^2 \ln\left[1 + e^{-\beta\left(\frac{\hbar^2 k^2}{2m} - \mu\right)}\right]$$

We apply partial integration:

$$\Omega_0 = (2S+1)\frac{V}{2\pi^2} \left[\left[\ln\left(1 + e^{-\beta \dots}\right) \frac{k^3}{3} \right]_0^{\infty} - \int_0^{\infty} dk \frac{k^3}{3} \frac{\partial}{\partial k} \left[\ln \dots \right] \right]$$

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

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

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

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.