Summary of Useful Z Equations

$$Z = \sum_{\text{ASN}} e^{-\varepsilon_i/kT} = \sum g_i e^{-\varepsilon_i/kT}$$

① get ε_i & g_i from Q.M.
② get $Z(T,V)$
③ get everything else from Z !!

$$U = -\frac{1}{Z}\frac{\partial Z}{\partial \beta} \quad \text{or} \quad U = -\frac{\partial \ln Z}{\partial \beta} \quad \text{or} \quad U = \frac{kT^2}{Z}\left(\frac{\partial Z}{\partial T}\right)_V$$

$$N_i = \left(\frac{N_{TOT}}{Z}\right) g_i e^{-\varepsilon_i/kT}$$

This is population of i^{th} level ε_i

$$F = -NkT \ln Z$$

Helmholtz Free Energy ("A" in UHAG)

$$P = -\left(\frac{\partial F}{\partial V}\right)_{T,N} = NkT\left(\frac{\partial \ln Z}{\partial V}\right)_{T,N}$$

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

$$C_V = \left(\frac{\partial U}{\partial T}\right)_V$$

"Ideal" Diatomic Gas:

$$Z = Z_{trans} \cdot Z_{rot} \cdot Z_{vib}$$

$$Z_{vib} = \left(\frac{e^{-h\nu/2kT}}{1 - e^{-h\nu/kT}}\right)$$

$kT \gg \varepsilon$ "classical" limit

$$Z_{rot} \simeq \left(\frac{kT}{\hbar^2/2I}\right)$$

e.g. $Z_{trans.} = \frac{V}{h^3}(2\pi mkT)^{3/2}$

For "N" identical, indistinguishable particles $\quad Z_{trans.} = \frac{1}{N!}\left(\frac{V}{v_Q}\right)^N$