Physics 410 -- Useful Formulas #1

0. Physical Constants

$N_A = 6.02\times10^{23}\,\text{mol}^{-1}$ $\quad k_B = 1.38\times10^{-23}\,\text{J/K}$ $\quad N_A k_B = 8.31\ \text{J/(mol - K)}$

$\hbar = 1.055\times10^{-34}$ J-s $\quad e = 1.60\times10^{-19}\,\text{C}$ $\quad m_p = 1.67\times10^{-27}\,\text{kg}$

Kittel and Kroemer notation: $\tau = k_B T$, $\sigma = S/k_B$

I. Probability and statistics, and other mathematical formulas:

mean value and variance: $\overline{X} \equiv \langle X\rangle = \sum_s X(s)P(s)$, $\langle(\Delta X)^2\rangle = \langle X^2\rangle - \langle X\rangle^2$

where P(s) is a normalized probability distribution: $\sum_s P(s) = 1$

binomial distribution: $(p+q)^N = \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} p^n q^{N-n}$

geometric series: $\sum_{n=0}^{N} x^n = \frac{1-x^{N+1}}{1-x}$, $\quad \sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$, for $|x|<1$

Stirling's approximation: $\ln(n!) \approx \frac{1}{2}\ln(2\pi) + (n+\frac{1}{2})\ln(n) - n$

binomial multiplicity for large N: $g(N,s) = \frac{N!}{(\frac{N}{2}+s)!(\frac{N}{2}-s)!} \approx \left(\frac{2}{\pi N}\right)^{1/2} 2^N e^{-2s^2/N}$

Gaussian integrals: $\int_{-\infty}^{\infty} e^{-x^2}\,dx = \sqrt{\pi}$ $\quad \int_{-\infty}^{\infty} x^2 e^{-x^2}\,dx = \frac{\sqrt{\pi}}{2}$

Normalized Gaussian probability distribution: $P(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\overline{x})^2}{2\sigma^2}}$

Taylor series: $f(x_0+\Delta x) = f(x_0) + f'(x_0)\Delta x + \frac{f''(x_0)}{2!}(\Delta x)^2 + \ldots$

examples: $\ln(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \ldots$ $\quad e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots$

II. Microcanonical ensemble: independent variables *U, V, N*

multiplicity function: $g(U,V,N)$; entropy: $\sigma(U,V,N) = \ln g(U,V,N)$

temperature: $\frac{1}{\tau} = \left(\frac{\partial\sigma}{\partial U}\right)_{V,N}$ pressure: $p = \tau\left(\frac{\partial\sigma}{\partial V}\right)_{U,N}$

Alternative formulation with independent variables σ, V, N

temperature: $\tau = \left(\frac{\partial U}{\partial\sigma}\right)_{V,N}$ pressure: $p = -\left(\frac{\partial U}{\partial V}\right)_{\sigma,N}$

III. Canonical ensemble: independent variables τ, *V, N*

Partition function: $Z = \sum e^{-\frac{\varepsilon_s}{\tau}}$, Canonical distribution function: $P_s = \frac{e^{-\frac{\varepsilon_s}{\tau}}}{Z}$

The numerator of P_s is called the "Boltzmann factor"

Partition function for a system of N identical subsystems or particles:

Distinguishable: $Z_N = (Z_1)^N$ indistinguishable, Classical limit: $Z_N = \frac{(Z_1)^N}{N!}$

Mean Energy: $U = \tau^2 \frac{\partial(\ln Z)}{\partial\tau} = -\frac{\partial(\ln Z)}{\partial\beta}$ where $\beta = \frac{1}{\tau}$

Helmholtz free energy: $F = U - \tau\sigma = -\tau\ln Z$

entropy: $\sigma = -\left(\frac{\partial F}{\partial\tau}\right)_{V,N}$ pressure: $p = -\left(\frac{\partial F}{\partial V}\right)_{\tau,N}$

heat capacity: $C_V = \left(\frac{\partial U}{\partial\tau}\right)_V = \tau\left(\frac{\partial\sigma}{\partial\tau}\right)_V$

IV. Thermodynamic Identity for systems with fixed N: $dU = \tau d\sigma - pdV = TdS - pdV$

For reversible processes: $dQ = \tau d\sigma$, $dW = pdV$, so $dU = dQ - dW$ for constant N

Compare 1st Law of Thermodynamics: $\Delta U = Q - W$, W is work done by the system.