Physics 410 – Final Exam equations

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: $(p+q)^N = \sum_{n=0}^{N} \frac{N!}{n!(N-n)!} p^n q^{N-n}$, or $g(N,n) = \frac{N!}{(n)!(N-n)!}$

geometric series: $\sum_{n=0}^{N} x^n = \frac{1-x^{N+1}}{1-x}$, $\sum_{n=0}^{\infty} x^n = \frac{1}{1-x}$, 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: $\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$ $\int_{-\infty}^{\infty} x^2 e^{-x^2} dx = \frac{\sqrt{\pi}}{2}$

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

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

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.

Heat engine efficiency: $\eta = \frac{W}{Q_h}$; Carnot efficiency $\eta_C = \frac{\tau_h - \tau_l}{\tau_h}$

Coefficient of refrigerator performance (CRP): $\gamma = \frac{Q_l}{W}$, Carnot CRP: $\gamma_C = \frac{\tau_l}{\tau_h - \tau_l}$

Ideal gas in 3D: $pV = N\tau$, $U = \frac{3}{2}N\tau$, $\sigma = N(\ln(n_Q/n) + 5/2)$

V. Chemical potential: $\mu_{total} = \mu_{int} + \mu_{ext}$, where μ_{int} depends on the particle density (e.g. through the Ideal Gas relation) and μ_{ext} is a potential energy per particle added to the system).

Diffusive equilibrium between systems A and B occurs when $\mu_{total}^A = \mu_{total}^B$

Chemical potential of ideal gas in 3D: $\mu = \tau \ln\left(\frac{n}{n_Q}\right)$, where n is the concentration of particles and $n_Q = \left(\frac{M\tau}{2\pi\hbar^2}\right)^{\frac{3}{2}}$ is the quantum concentration.

VI. Grand canonical ensemble: independent variables τ, V, μ

Grand Partition function, also called the "Gibbs sum": $\zeta = \sum_{ASN} e^{(N\mu - \epsilon_s)/\tau}$, where $\sum_{ASN}$ indicates a sum over all states and number of particles.

Grand canonical distribution function (probability): $P(N, \epsilon) = \frac{e^{\frac{(N\mu - \epsilon)}{\tau}}}{\zeta}$

The numerator of $P(N,\varepsilon)$ is called the "Gibbs factor"

Mean number of particles: $\langle N \rangle = \lambda \frac{d(\ln \zeta)}{d\lambda}$, where $\lambda = e^{\mu/\tau}$

VIII. Fermi gas. Fermi-Dirac distribution function: $f(\epsilon) = \frac{1}{e^{\frac{\epsilon - \mu}{\tau}} + 1}$

At $\tau = 0$, $f(\epsilon) = 1$ for $\epsilon < \epsilon_F$ and $f(\epsilon) = 0$ for $\epsilon > \epsilon_F$

Thermal averages via distribution function:
$\langle X \rangle = \sum_{\text{orbitals}} X f(\epsilon) = \int_0^\infty X\, D(\epsilon)\, f(\epsilon)\, d\epsilon$, where $D(\epsilon)$ is the density of states

Total number of particles: $N = \sum_{\text{orbitals}} f(\epsilon) = \int_0^\infty D(\epsilon)\, f(\epsilon)\, d\epsilon$

Ideal gas: classical regime of Fermi-Dirac and Bose-Einstein distributions, with $f(\epsilon) = e^{\frac{\mu - \epsilon}{\tau}}$.