Information Theory

Missing Information:

$$S = -k \sum_{i=1}^{r} p_i \ln p_i$$

Expectation values:

$$\overline{E} = \sum_i E_i p_i$$

Canonical Ensemble:

$$p_i = \frac{1}{Z_c} e^{-\beta E_i} \qquad \text{where} \qquad Z_c = \sum_i e^{-\beta E_i}$$

Grand-Canonical Ensemble:

$$p_{i,N} = \frac{1}{Z_{gc}} e^{-\beta(E_{iN} - N\mu)}$$

$$\text{where} \qquad Z_c = \sum_i e^{-\beta(E_{iN} - N\mu)}$$

Thermodynamics

Potentials:

$$F = \overline{E} - TS$$

$$H = \overline{E} + PV$$

$$G = \overline{E} - TS + PV$$

$$\Phi = F - \overline{N}\mu = \overline{E} - TS - \mu\overline{N}$$

Bridge Equations:

$$F = -kT \ln Z_c$$

$$\Phi = -kT \ln Z_{gc}$$

$$\overline{E} = -\frac{1}{Z_c}\frac{\partial Z_c}{\partial \beta} = -\frac{\partial \ln Z_c}{\partial \beta}$$

Fluctuations

$$\Delta E_i = E_i - \overline{E}$$

$$\overline{(\Delta E)^2} = \overline{E^2} - \overline{E}^2$$

$$\Delta E_{rms} = \overline{\Delta E^2}^{\frac{1}{2}}$$

$$\text{relative fluctuation} = \frac{\Delta E_{rms}}{\overline{E}}$$

Weakly Interacting Constituents

Localised particles (distinguishable):

$$Z_c = [Z(1)]^N \qquad \text{where} \qquad Z(1) = \sum_i e^{-\beta\epsilon_i}$$

Non localised (Fermi-Dirac):

$$Z_{gc} = \prod_j Z_j \qquad \text{where} \qquad Z_j = \sum_{n_j} e^{\beta n_j(\mu - \epsilon_j)}$$

Fermi-Dirac Statistics:

$$Z_j = (1 \pm e^{\beta(\mu - \epsilon_j)})^{\pm 1} \text{ for } \begin{cases} + \text{ Fermions} \\ - \text{ Bosons} \end{cases}$$

$$\overline{n_j} = \frac{1}{e^{\beta(\epsilon_j - \mu)} \pm 1} \text{ for } \begin{cases} + \text{ Fermions} \\ - \text{ Bosons} \end{cases}$$

Geometric Series:

$$\sum_{n=0}^{\infty} x^n = \frac{1}{1-x} \qquad \text{for } |x| < 1$$

B-E Condensation

Density of States:

$$g(\epsilon) = \left(\frac{2m}{\hbar^2}\right)^{\frac{2}{3}} \frac{V}{4\pi^2} \epsilon^{\frac{1}{2}} \equiv AV\epsilon^{\frac{1}{2}}$$

Critical Density:

$$\rho_c(T) = A\frac{\sqrt{\pi}}{2}\zeta(3/2)(kT)^{\frac{3}{2}}$$

$$\rho = \rho_o + \rho_+ = \frac{1}{V}\frac{1}{e^{-\beta\mu} - 1} + A\int_0^{\infty} \frac{\epsilon^{\frac{1}{2}}}{e^{\beta(\epsilon - \mu)} - 1} d\epsilon$$

Thermal Wavelength:

$$\lambda_T = \left(\frac{2\pi\hbar^2}{mkT}\right)^{\frac{1}{2}}$$

Condensation Condition:

$$\left(\frac{V}{\overline{N}}\right)^{\frac{1}{3}} = \rho_c^{-\frac{1}{3}} \sim \lambda_T \ll \text{ interparticle spacing}$$

Particle in a Box Energy Levels:

$$\epsilon = \frac{\hbar^2\pi^2}{2mL^2}(n_x^2 + n_y^2 + n_z^2) + \text{ constant}$$

Debye Model

Density of States:

$$g(\omega) = 3\frac{V}{2\pi^2}\frac{\omega^2}{c_s^3} \equiv AV\omega^2$$

Cutoff Frequency:

$$\omega_{max} = \left(6\pi^2\frac{N}{V}\right)^{\frac{1}{3}} c_s$$

$$k\Theta_D = \hbar\omega_{max}$$

Ideal Gas Perturbations

Basics

Canonical partition function as integral in 6N-dimensional phase space:

$$Z_c = \frac{1}{N!h^{3N}} \int \prod_i d^3q_i d^3p_i \exp[-\beta H(\{\vec{q}\}, \{\vec{p}\})]$$

$$Z_c = Z_{ideal} Q \quad \text{where} \quad Z_{ideal} = \frac{1}{N!} \left[\frac{V}{\lambda_T^3}\right]^N$$

configuration integral:

$$Q = V^{-N} \int \prod_{i=1}^N d^3q_i e^{-\beta U(\vec{q_1} \dots \vec{q_N})}$$

Virial Expansion

2-body interactions and central potential:

$$U(\{\vec{q}\}) = \sum_{i<j} \phi_{ij}$$

Spatial average configuration integral:

$$Q = \frac{1}{V^N} \int \prod_i d^3q_i \prod_{i<j} F_{ij} \approx \langle F \rangle^{N(N-1)/2}$$

$$\langle F_{12} \rangle = 1 - \frac{2B_2}{V}$$

second virial coefficient:

$$B_2 = -\frac{1}{2} \int d^3r (e^{-\beta\phi(r)} - 1)$$

Equation of State:

$$\frac{P}{kT} = \rho + B_2\rho^2$$

Reduced Density Distributions

Distribution function for any set of m particles occupying stated positions:

$$\rho_m(\vec{r_1}, ..., \vec{r_m}) = \frac{N!}{(N-m)!} \int p(\vec{r_1}, ..., \vec{r_N}) \prod_{i=m+1}^N d^3r_i$$

$$\rho_2(\vec{r_1}, \vec{r_2}) = \rho^2 g(|\vec{r_1} - \vec{r_2}|)$$

With radial distribution function $g(r)$

$$\int d^3r \rho g(r) = N \qquad \text{and also} \qquad \int d^3r g(r) = V$$

Virial equation of state:

$$P = \rho kT - \frac{\rho^2}{6} \int_0^\infty \left(r\frac{d\phi}{dr}\right) g(r) 4\pi r^2 dr$$

Debye-Hückel Theory

Poisson's Equation:

$$\nabla^2\phi(r) = -\frac{\rho(r)}{\epsilon}$$

Debye-Hückel equation:

$$\nabla^2\phi - \frac{\phi}{\lambda_D^2} = -\frac{q}{\epsilon}\delta(\vec{r})$$

Debye screening length:

$$\lambda_D = \left(\frac{kT\epsilon}{q^2 n_\infty}\right)^{1/2}$$

Solution for potential:

$$\phi(r) = A\frac{e^{-r/\lambda_D}}{r}$$