# **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:

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

Grand-Canonical Ensemble:

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

where 
$$Z_c = \sum_{i} e^{-\beta(E_{iN} - N\mu)}$$

## 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**

$$\Delta E_i = E_i - \overline{E}$$
$$\overline{(\Delta E)^2} = \overline{E^2} - \overline{E}^2$$
$$\Delta E_{rms} = \overline{\Delta E^2}^{\frac{1}{2}}$$

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

# Weakly Interacting Constituents

Localised particles (distinguishable):

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

Non localised (Fermi-Dirac):

$$Z_{gc} = \prod_{j} Z_{j}$$
 where  $Z_{j} = \sum_{n_{j}} e^{\beta n_{j}(\mu - \epsilon_{j})}$ 

Fermi-Dirac Statistics:

$$Z_j = (1 \pm e^{\beta(\mu - \epsilon_j)})^{\pm 1}$$
 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:

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

### **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:

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

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:

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

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:

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

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

configuration integral:

$$Q = V^{-N} \int \prod_{i=1}^{N} d^{3}q_{i} e^{-\beta U(\vec{q_{1}}...\vec{q_{N}})}$$

## Virial Expansion

2-body interactions and central potential:

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

Spatial average configuration integral:

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

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

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:

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

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

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:

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

## Ising Model

Configurational energy:

$$E(\lbrace S_i \rbrace) = -h \sum_{i} S_i - J \sum_{\langle ij \rangle} S_i S_j$$

Mean field approximation:

$$\epsilon_{mf} \approx -hS_j - JS_j \sum_{k}^{\pm nn} \langle S_k \rangle = -h_{mf}S_j$$

where

$$h_{mf} = h + Jzm$$

Spin  $\pm$  1 magnetisation (order paramater):

$$m = \tanh(\beta h + \beta Jzm)$$

Critical Temp:

$$T_c = \frac{zJ}{k}$$

### **Exact Results**