

1 Introduction to probability theory

Bayes' theorem

$$p(B|A)=\frac{p(A|B)\cdot p(B)}{p(A)}=\frac{p(A|B)\cdot p(B)}{\sum_{B'}p(A|B)\cdot p(B')}$$

Expactation and covariance

$$\langle f \rangle = \sum_i f(i)p_i \text{ or } \langle f \rangle = \int f(x)p(x)dx$$

$$\mu = \langle i \rangle = \sum_i i p_i \text{ or } \mu = \langle x \rangle = \int x p(x) dx$$

$$\sigma^2 = \langle i^2 \rangle - \langle i \rangle^2$$

$$\sigma_{ij}^2 = \langle ij \rangle - \langle i \rangle \langle j \rangle$$

Binomial distribution

$$\frac{N!}{(N-i)!i!} = \binom{N}{i} \text{ binomial coefficient}$$

$$p_i = \binom{N}{i} \cdot p^i q^{N-i} \text{ distribution}$$

$$\mu = \langle i \rangle = N \cdot p$$

$$\langle i^2 \rangle = p \cdot N + p^2 \cdot N \cdot (N-1)$$

$$\sigma^2 = N \cdot p \cdot q$$

$$\sum_{i=0}^N p_i = \sum_{i=0}^N \binom{N}{i} \cdot p^i q^{N-i} = (p+q)^N = 1$$

Gauss distribution

$$p(x) = \frac{1}{\left(2\pi\sigma^2\right)^{\frac{1}{2}}} \cdot e^{-\frac{x-\mu}{2\sigma^2}}, \quad \langle x^2 \rangle = \sigma^2$$

Poisson distribution

$$p(k;\mu) = \frac{\mu^k}{k!} e^{-\mu}, \quad E[k] = \mu, \quad V[k] = \mu$$

Information entropy

$$S = - \sum_i p_i \ln(p_i)$$

2 The microcanonical ensemble

$E \approx \text{const}$, $V = \text{const}$, $N = \text{const}$.

The fundamental postulate

$$\Omega(E) = \sum_{n:E-\delta E \leq E_n \leq E} 1$$

$$\Omega(E;\delta E) = \frac{1}{h^{3N} N!} \iint_{E-\delta E \leq \mathcal{H}(\vec{q},\vec{p}) \leq E} d\vec{q} d\vec{p}$$

$$S = -k_B \sum_{i=1}^{\Omega} p_i \ln(p_i) = k_B \ln(\Omega)$$

n_0 different particles

$$\Omega = \frac{1}{h^{3N} \prod_{j=0}^{n_0} N_j!} \iint_{E-\delta E \leq \mathcal{H}(\vec{q},\vec{p}) \leq E} d\vec{q} d\vec{p}$$

Equilibrium conditions

Entropy S must be maximal

Thermal contact

$$\left. \frac{\partial S(E,V,N)}{\partial E} \right|_{V,N} = \frac{1}{T(E,V,N)}$$

Contact with volume exachnge

$$\left. \frac{\partial S(E,V,N)}{\partial V} \right|_{E,N} = \frac{p(E,V,N)}{T(E,V,N)}$$

Contact with exchange of particle number

$$\left. \frac{\partial S(E,V,N)}{\partial N} \right|_{E,V} = - \frac{\mu(E,V,N)}{T(E,V,N)}$$

Equations of state

$$dE = T dS - p dV + \mu dN$$

Specific heat

$$c_v = \frac{dE}{dT}$$

solution concept

- Set up Hamiltonian
- Calculate phasevolume Ω
- Calculate entropy S
- determine T, p, μ
- Calculate $U = \langle E \rangle$
- thermodynamic potentials:
 $F(T,V,N) = U - TS$
 $\dot{H}(S,p,N) = U + pV$
 $G(T,p,N) = U + pV - TS$

Ideal Gas

$$\mathcal{H} = \sum_{i=1}^{3N} \frac{p_i^2}{2m} + V(q_1, \dots, q_{3N})$$

microcanonical partition sum for an ideal gas

$$\Omega(E) = \frac{V^N \pi^{3N/2} (2mE)^{3N/2}}{h^{3N} N! \left(\frac{3N}{2}\right)!}$$

$$S = k_B N \left\{ \ln \left[\left(\frac{V}{N} \right) \left(\frac{4\pi m E}{3h^2 N} \right)^{3/2} \right] + \frac{5}{2} \right\}$$

Equations of state fo ideal gas

$$\frac{1}{T} = \left(\frac{\partial S}{\partial E} \right)_{N,V} = \frac{3}{2} \frac{N k_B}{E} \rightarrow U = \frac{3}{2} N k_B T$$

$$p = T \left(\frac{\partial S}{\partial V} \right)_{E,N} = T N k_B \frac{1}{V} \rightarrow pV = N k_B T$$

$$\mu = k_B T \ln \left(\frac{N \lambda^3}{V} \right) \text{ chemical potential}$$

$$\lambda = \frac{h}{\sqrt{2\pi m k_B T}} \text{ Thermal de Broglie}$$

Einstein model for specific heat of a solid

$$E = \hbar \omega \left(\frac{N}{2} + Q \right) \rightarrow Q = \left(\frac{E}{\hbar \omega} - \frac{N}{2} \right)$$

$$\Omega(E,N) = \frac{(Q+N)!}{Q!N!}$$

$$S = k_B \left[Q \ln \left(\frac{Q+N}{Q} \right) + N \ln \left(\frac{Q+N}{N} \right) \right]$$

$$= k_B N \left[\left(e + \frac{1}{2} \right) \ln \left(e + \frac{1}{2} \right) - \left(e - \frac{1}{2} \right) \ln \left(e - \frac{1}{2} \right) \right]$$

$$e = E/E_0 ; E_0 = N \hbar \omega ; \beta = \hbar \omega / k_B T$$

$$\frac{1}{T} = \frac{\partial S}{\partial E} \Rightarrow E = N \hbar \omega \left(\frac{1}{2} + \frac{1}{e^\beta - 1} \right)$$

Entropic elasticity of polymers

$$N_+ - N_- = \frac{L}{a} = m \rightarrow N_+ = \frac{1}{2} (N + m)$$

$$\Omega = \frac{N!}{N_+! N_-!} = \frac{N!}{\left(\frac{1}{2}(N+m)\right)! \left(\frac{1}{2}(N-m)\right)!}$$

if both directions are possible x_2

$$S = -k_B \left(N_+ \ln \left(\frac{N_+}{N} \right) + N_- \ln \left(\frac{N_-}{N} \right) \right)$$

Statistical deviation from average

Two ideal gases in thermal conact $T_1 = T_2$

$$S_i = \frac{3}{2} k_B N_i \ln(E_i) + \text{independent of } E_i$$

$$S = S_1 + S_2$$

$$dS = 0 \rightarrow \frac{\partial S_1}{\partial E_1} = \frac{\partial S_2}{\partial E_2}$$

$$\rightarrow \bar{E}_1 = \frac{N_1}{N} E$$

consider small deviation:

$$E_1 = \bar{E}_1 + \Delta E, \quad E_2 = \bar{E}_2 - \Delta E$$

$$S(\bar{E}_1 + \Delta E) \approx \frac{3}{2} k_B \left[N_1 \ln \bar{E}_1 + N_2 \ln \bar{E}_2 \right.$$

$$\left. - \frac{N_1}{2} \left(\frac{\Delta E}{\bar{E}_1} \right)^2 - \frac{N_2}{2} \left(\frac{\Delta E}{\bar{E}_2} \right)^2 \right]$$

$$\rightarrow \Omega = \bar{\Omega} e^{\left[-\frac{3}{4} \left(\frac{\Delta E}{\bar{E}} \right)^2 N^2 \left(\frac{1}{N_1} + \frac{1}{N_2} \right) \right]}$$

3 The canonical ensemble

$T = \text{const}$, $V = \text{const}$, $N = \text{const}$.

Boltzmann distribution

$$p_i = \frac{1}{Z} e^{-\beta E_i} \quad \text{Boltzmann distribution}$$

$$Z = \sum_i e^{-\beta E_i} \quad \text{partition sum}$$

For classical Hamiltonian systems:

$$p(\vec{q},\vec{p}) = \frac{1}{Z N! h^{3N}} e^{-\beta \mathcal{H}(\vec{q},\vec{p})}$$

$$Z_N(T,V) = \frac{1}{N! h^{3N}} \iint d\vec{q} d\vec{p} e^{-\beta \mathcal{H}(\vec{q},\vec{p})}$$

For common Hamiltonian:

$$Z_N(T,V) = \frac{1}{\lambda^{3N} N!} \int_V d\vec{q} e^{-\beta \hat{V}(\vec{q})}$$

Free energy

$$F(T,V,N) = -k_B T \ln Z_N(T,V)$$

$$\langle E \rangle = U = -\partial_\beta \ln Z_N$$

total differential:

$$dF = dE + d(TS) = -S dT - p dV + \mu N$$

equations of state

$$S = -\frac{\partial F}{\partial T}, \quad p = -\frac{\partial F}{\partial V}, \quad \mu = \frac{\partial F}{\partial N}$$

Non-interacting systems

ϵ_{ij} is the j^{th} state of the i^{th} element

$$Z = \sum_{j_1} \sum_{j_2} \dots \sum_{j_N} e^{-\beta \sum_{i=1}^N \epsilon_{ij_i}}$$

$$= \left(\sum_{j_1} e^{-\beta \epsilon_{1j_1}} \right) \dots \left(\sum_{j_N} e^{-\beta \epsilon_{Nj_N}} \right)$$

$$= z_1 \cdot \dots \cdot z_N = \prod_{i=1}^N z_i$$

$$\rightarrow F = -k_B T \sum_{i=1}^N \ln(z_i) = -k_B T \ln(Z)$$

$$Z = z^N, \quad F = -k_B T N \ln(z)$$

Ideal Gas

$$\mathcal{H} = \sum_{i=1}^N \frac{\vec{p}_i^2}{2m}$$

$$Z_N(T,V) = \frac{V^N}{N!} \left(\int_{-\infty}^{+\infty} \frac{dp}{h} e^{-\beta \frac{p^2}{2m}} \right)^{3N} \\ = \frac{1}{N!} \left(\frac{V}{\lambda^3} \right)^N$$

Equipartition theorem

f_{dof} are the degrees of freedom.

harmonic Hamiltonian with $f_{dof} = 2$

$$\mathcal{H} = A q^2 + B p^2$$

$$z \propto \int dq dp e^{-\beta \mathcal{H}}$$

$$= \left(\frac{\pi}{A\beta} \right)^{\frac{1}{2}} \cdot \left(\frac{\pi}{B\beta} \right)^{\frac{1}{2}} \propto \left(T^{\frac{1}{2}} \right)^{f_{dof}}$$

For sufficiently high temperture (classical limit), each quadratic term in the Hamiltonian contributes a factor $T^{\frac{1}{2}}$ to the partition

sum ('equipartition theorem')

$$F = -k_B T \ln(z) = -\frac{f_{dof}}{2} k_B T \ln(T)$$

$$S = -\frac{\partial F}{\partial T} = \frac{f_{dof}}{2} k_B (\ln(T) + 1)$$

$$U = -\partial_\beta \ln(z) = \frac{f_{dof}}{2} k_B T$$

$$c_v = \frac{dU}{dT} = \frac{f_{dof}}{2} k_B$$

$$c_p = \frac{f_{dof} + 2}{2} k_B$$

Molecular gases

N molecules; x different mode types:

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

$$Z_x = z_x^N$$

Vibrational modes

often described by the Morse potential:

$$V(r) = E_0 \left(1 - e^{-\alpha(r-r_0)} \right)^2$$

An exact solution of the Schrödinger equation gives:

$$E_n = \hbar \omega_0 \left(n + \frac{1}{2} \right) - \frac{\hbar^2 \omega_0^2}{e E_0} \left(n + \frac{1}{2} \right)^2$$

$$\omega_0 = \frac{\alpha}{2\pi} \sqrt{\frac{2E_0}{\mu}}, \quad \mu = \frac{m}{2}$$

For $\hbar \omega_0 \ll E_0$ we can use the harmonic approximation:

$$z_{vib} = \frac{e^{-\beta \hbar \omega_0 / 2}}{1 - e^{-\beta \hbar \omega_0}}$$

$$T_{vib} \approx \frac{\hbar \omega_0}{k_B} \approx 6.140 K \text{ for } H_2$$

Rotational modes

standart approximation is the one of a rigid rotator. The moment of inertia is given as:

$$I = \mu r_0^2 \quad T_{rot} = \frac{\hbar^2}{I k_B} \quad \omega_n = (2J + 1)$$

$$\rightarrow E_l = \frac{\hbar^2}{2I} l(l+1)$$

Nuclear contributions: ortho- and parahydrogen

$$S = 1, z_{ortho} = \sum_{l=1,3,5,\dots} (2l+1) e^{-\frac{l(l+1)T_{rot}}{T}}$$

$$S = 0, z_{para} = \sum_{l=0,2,4,\dots} (2l+1) e^{-\frac{l(l+1)T_{rot}}{T}}$$

Specific heat of a solid

Debye model

$$\rightarrow \omega(k) = \left(\frac{4\kappa}{m}\right)^{\frac{1}{2}} \left| \sin\left(\frac{ka}{2}\right) \right|$$

$$\omega = \frac{2\pi}{T}, \quad k = \frac{2\pi}{\lambda}$$

Debye frequency:

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

$$c_s = \left. \frac{d\omega}{dk} \right|_{k=0} = \sqrt{\frac{\kappa}{m}} a$$

density of states in ω -space:

$$D(\omega) = 3 \frac{\omega^2}{\omega_D^3} \quad \text{for } \omega \leq \omega_D$$

count modes in frequency-space:

$$\sum_{modes} (...) = 3 \sum_k (...) = 3N \int_0^{\omega_D} d\omega D(\omega) (...)$$

partition sum:

$$z(\omega) = \frac{e^{-\beta \hbar \omega / 2}}{1 - e^{-\beta \hbar \omega}}$$

$$\rightarrow Z = \prod_{modes} z(\omega)$$

$$\rightarrow E = -\partial_\beta \ln(Z) = \sum_{modes} \hbar \omega \left(\frac{1}{e^{\beta \hbar \omega} - 1} + \frac{1}{2} \right)$$

$$= E_0 + 3N \int_0^{\omega_D} d\omega \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1} \frac{3\omega^2}{\omega_D^3}$$

$$c_v(T) = \frac{\partial E}{\partial T}$$

$$= \frac{3\hbar^2 N}{k_B T^2} \int_0^{\omega_D} d\omega \frac{3\omega^2}{\omega_D^3} \frac{e^{\beta \hbar \omega} \omega^2}{(e^{\beta \hbar \omega} - 1)^2}$$

$$u = \beta \hbar \omega$$

$$c_v(T) = \frac{9Nk_B}{u_m^3} \int_0^{u_m} \frac{e^u u^4}{(e^u - 1)^2} du$$

the limit for $\hbar \omega_D \ll k_B T$:

$$c_v(T) = 3Nk_B$$

the limit for $k_B T \ll \hbar \omega_D$: ($T_D = \frac{\hbar \omega_D}{k_B}$)

$$c_v(T) = \frac{12\pi^4}{5} Nk_B \left(\frac{T}{T_D} \right)^3$$

Black body radiation

$$E = \frac{4\sigma}{c} VT^4, \quad \sigma = \frac{\pi^2 k_B^4}{60\hbar^3 c^2}$$

$$c_v = \frac{16\sigma}{c} VT^3$$

$$J = \frac{P}{A} = \sigma T^4 \quad \text{Stefan- Boltzmann law}$$

Plank's law for black body radiation

$$u(\omega) := \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{e^{\hbar \omega / (k_B T)} - 1}$$

The Plank distribution has a maximum at:
 $\hbar \omega_{max} = 2.82 k_B T$ Wien's displacement law

4 The grandcanonical ensemble

$T, \mu = const.$

$$p_N(q, p) = \frac{1}{\Xi_\mu(T, V)} e^{-\beta(H_N(q, p) - \mu N)}$$

$$\Xi_\mu(T, V) = \sum_{N=0}^{\infty} \frac{1}{h^{3N} N!} \iint d^{3N} q d^{3N} p e^{-\beta(H_N - \mu N)}$$

$$\rightarrow \Xi_z = \sum_{N=0}^{\infty} z^N Z_N(T, V)$$

$z = e^{\beta \mu} \rightarrow$ Fugacity

Mean phase space observable

$$\langle F \rangle = \frac{1}{\Xi_\mu(T, V)} \sum_{N=0}^{\infty} \frac{1}{h^{3N} N!} \iint d^{3N} q d^{3N} p \dots$$

$$\dots e^{-\beta(H_N - \mu N)} F_N(q, p)$$

mean particle number:

$$\langle N \rangle = \frac{1}{\beta} \left(\frac{\partial}{\partial \mu} \ln(\Xi_\mu(T, V)) \right)_{T, V}$$

$$= z \left(\frac{\partial}{\partial z} \ln(\Xi_z(T, V)) \right)_{T, V}$$

pressure:

$$p = - \left\langle \frac{\partial H}{\partial V} \right\rangle = \frac{1}{\beta} \left(\frac{\partial}{\partial V} \ln(\Xi_\mu(T, V)) \right)$$

energy U :

$$U = \langle H \rangle = - \left(\frac{\partial}{\partial \beta} \ln(\Xi_\mu(T, V)) \right)_{\mu, V} + \mu \langle N \rangle$$

$$= - \left(\frac{\partial}{\partial \beta} \ln(\Xi_z(T, V)) \right)_{z, V}$$

Grandcanonical potential

grandcanonical potential:

$$\Psi(T, V, \mu) = -k_B T \ln(\Xi_\mu(T, V))$$

p is maximal, if Ψ is minimal.

Total differential:

$$d\Psi = -SdT - pdV - \langle N \rangle d\mu$$

Equations of state:

$$S = -\frac{\partial \Psi}{\partial T}, p = -\frac{\partial \Psi}{\partial V}, N = -\frac{\partial \Psi}{\partial \mu}$$

Fluctuations

$$\sigma_N^2 = \langle N^2 \rangle - \langle N \rangle^2 = \frac{1}{\beta^2} \left(\partial_\mu^2 \ln(\Xi_\mu) \right)$$

$$\frac{\sigma_N}{\langle N \rangle} \propto \frac{1}{\sqrt{N}}$$

Ideal gas

$$Z_N(T, V) = \frac{1}{N!} \left(\frac{V}{\lambda^3} \right)^N, \quad \lambda = \frac{h}{(2\pi m k_B T)^{\frac{1}{2}}}$$

$$\Xi = \sum_{N=0}^{\infty} Z_N(T, V) z^N$$

$$= \sum_{N=0}^{\infty} \frac{1}{N!} \left(e^{\beta \mu} \frac{V}{\lambda^3} \right)^N$$

$$= e^{z \frac{V}{\lambda^3}} \quad \text{fugacity: } z := e^{\beta \mu}$$

$$\langle N \rangle = \frac{1}{\beta} \partial_\mu \ln(Z_G) = \frac{V}{\lambda^3} d^{\beta \mu}$$

$$\mu = k_B T \ln \left(\frac{N \lambda^3}{V} \right)$$

Molecular adsorption onto a surface

$$Z_G = z_G^N; z_G = 1 + e^{-\beta(\epsilon - \mu)}$$

$$\langle n \rangle = \frac{1}{e^{-\beta(\mu - \epsilon)} + 1} \quad \text{per site}$$

$$\langle \epsilon \rangle = \epsilon \langle n \rangle$$

5 Quantum fluids

Fermion vs. bosons

1. Fermions: Pauli-principle + not distinguishable
2. Bosons: symmetric wave function + not distinguishable
3. Boltzmann: particles are distinguishable

Canonical ensemble

$\omega_n \rightarrow$ degeneracy of state n

$$z = \sum_n \omega_n \exp(-\beta E_n)$$

Grand canonical ensemble

only two states 0, ϵ

Fermions:

$$z_F = 1 + e^{-\beta(\epsilon - \mu)}$$

average occupation number n_F :

$$n_F = \frac{1}{e^{\beta(\epsilon - \mu)} + 1} \quad \text{Fermi function}$$

For $T \rightarrow 0$, the fermi function approaches a step function:

$$n_F = \Theta(\mu - \epsilon)$$

Bosons:

$$z_B = \frac{1}{1 - e^{-\beta(\epsilon - \mu)}}$$

average occupation number n_B :

$$n_B = \frac{1}{e^{\beta(\epsilon - \mu)} - 1}$$

- Fermions tend to fill up energy states one after the other
- Bosons tend to condense all into the same low energy state

The ideal Fermi fluid

density of states:

$$D(\epsilon) = \frac{V}{2\pi N} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \sqrt{\epsilon}$$

Fermi energy

$$N = \sum_{\vec{k}, m_s} n_{\vec{k}, m_s}^F = N \int_0^\infty d\epsilon D(\epsilon) n_F(\epsilon)$$

Limit $T \rightarrow 0$. $\mu(T=0)$ is called Fermi energy:

$$\epsilon_F = (3\pi^2)^{\frac{2}{3}} \frac{\hbar^2 \rho^{\frac{2}{3}}}{2m}$$

specific heat

$$\mu = \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\epsilon_F} \right)^2 \right] \quad \text{for } T \ll \frac{\epsilon_F}{k_B}$$

$$c_V = \left. \frac{\partial E}{\partial T} \right|_V = N \frac{\pi^2}{3} k_B^2 D(\epsilon_F) T$$

$$c_V = N \frac{\pi^2}{2} \frac{k_B T}{\epsilon_F} k_B$$

Fermi pressure

$$p \xrightarrow{T \rightarrow 0} \frac{2}{5} \frac{N}{V} \epsilon_F = \frac{(2\pi^2)^{\frac{2}{3}}}{5} \frac{\hbar^2}{m v^{\frac{5}{3}}}$$

The ideal Bose fluid

$\epsilon = \frac{\hbar^2 k^2}{2m}$ and conserved particle number N.

$$N = \frac{N}{\lambda^3} g_{\frac{3}{2}}(z)$$

$$z = e^{\beta \mu}, \quad \lambda = \frac{h}{(2\pi m k_B T)^{\frac{1}{2}}}$$

$$T_c = \frac{2\pi}{\left(\zeta\left(\frac{3}{2}\right) \right)^{\frac{3}{2}}} \frac{\hbar^2 \rho^{\frac{2}{3}}}{k_B m}$$

$$E = \frac{3}{2} k_B T \frac{V}{\lambda^3} g_{\frac{5}{2}}(z) = \frac{3}{2} k_B T N e^{\frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)}}$$

$$c_V = \frac{15}{4} k_B N \left(\frac{T}{T_c} \right)^{\frac{3}{2}} \frac{\zeta\left(\frac{5}{2}\right)}{\zeta\left(\frac{3}{2}\right)} \quad (\text{for } T \leq T_c)$$

$$c_V = \frac{15}{4} k_B N \frac{g_{\frac{5}{2}}(z)}{g_{\frac{3}{2}}(z)} - \frac{9}{4} k_B N \frac{g_{\frac{3}{2}}(z)}{g_{\frac{1}{2}}(z)} \quad (T > T_c)$$

Classical limit

$\mu \rightarrow -\infty$ the two grandcanonical distr. become the Maxwell-Boltzmann distr.

$$n_{F/B} = \frac{1}{e^{\beta(\epsilon - \mu)} \pm 1} \rightarrow e^{\beta \mu} e^{-\beta \epsilon}$$

$$N = g \frac{V}{\lambda^3} e^{\beta \mu}$$

$$E = \frac{3}{2} k_B T N$$

6 Phase transitions

Ising model

Hamiltonian

$$\mathcal{H} = - \sum_{i,j} J_{ij} S_i S_j - \mu B_0 \sum_i S_i$$

special cases:

Ferromagnetic systems:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{J}_i \vec{J}_j - \vec{\mu} \vec{B} \sum_i \vec{J}_i$$

lattice gases:

$$\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j$$

1. Dimensional

Only Next Neighbor and $B_0 = 0$

$$J_{i,i+1} \rightarrow J_i, \quad \mathcal{H} = - \sum_{i=1}^{N-1} J_i S_i S_{i+1}, \quad j_i = \beta J_i$$

$$Z_N = \sum_{S_1} \dots \sum_{S_N} \exp \left(\sum_{i=1}^{N-1} j_i S_i S_{i+1} \right)$$

$$= 2^N \prod_{i=1}^{N-1} \cosh(\beta J_i)$$

Spin correlation function:

$$\langle S_i S_{i+1} \rangle = \tanh(\beta J)$$

spontaneous magnetisation:

$$M_S(T) = \mu \langle S \rangle$$

$$M_S^2(T) = \mu^2 \lim_{j \rightarrow \infty} \langle S_i S_{i+1} \rangle$$

No phase transition for $T > 0$. But for $T = 0$

$$M_S(T=0) = \mu$$

Transfer matrix

$$j = \beta J, \quad b = \beta \mu B_0, \quad S_i = \pm 1$$

$$T_{i,i+1} = e^{j S_i S_{i+1} + \frac{1}{2} b (S_i + S_{i+1})}$$

$$\rightarrow e^{-\beta \mathcal{H}} = T_{1,2} \cdot T_{2,3} \dots T_{N,1}$$

$$T = \begin{pmatrix} T(+1,+1) & T(+1,-1) \\ T(-1,+1) & T(-1,-1) \end{pmatrix}$$

$$Z_N = \lambda_1^N + \lambda_2^N = E_+^N + E_-^N$$

for $N \gg 1 \rightarrow E_+ \gg E_-$

Renormalization of the Ising chain

$$K' = \frac{1}{2} \ln(\cosh(2K))$$

Renormalization of the 2d Ising model

$$\bar{K}' = K' + K_1 = \frac{3}{8} \ln(\cosh(4K))$$

The 2d Ising model

$$\beta \mathcal{H} = -K \sum_{r,c} S_{r,c} S_{r+1,c} - K \sum_{r,c} S_{r,c} S_{r,c+1}$$
$$1 = \sinh(2K_c)$$
$$K_c = \frac{1}{2} \ln \left(1 + \sqrt{2} \right) \approx 0.4407$$
$$T_c = 2J / \ln \left(1 + \sqrt{2} \right) \approx 2.269 J / k_B$$

Perturbation theory

$$F \leq F_u = F_0 + \langle \mathcal{H}_1 \rangle_0$$
Bogoliubov inequality

Mean field theory for the Ising model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} S_i S_j$$
$$\mathcal{H}_0 = -B \sum_i S_i$$
$$F_0 = -N k_B T \ln \left(e^{\beta B} + e^{-\beta B} \right)$$
$$= -N k_B T \ln (2 \cosh(\beta B))$$
$$F \leq F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0$$
$$= -N k_B T \ln (2 \cosh(\beta B)) - N \frac{z}{2} \langle S \rangle_0^2$$
$$+ N \langle S \rangle_0 = F_u$$
$$\rightarrow z = 2 \cdot \text{dimension}$$
$$B = J z \langle S \rangle_0 = J z \tanh(\beta B)$$

$$K_c = \frac{1}{z} \rightarrow T_c = \frac{zJ}{k_B}$$

7 Classical fluids

Virial expansion

$$F = N k_B T \left[\ln(\rho \lambda^3) - 1 + B_2 \rho \right]$$
$$p = \rho k_B T \left[1 + B_2 \rho \right]$$

Second virial coefficient

$$B_2(T) = -2\pi \int r^2 dr \left(e^{-\beta U(r)} - 1 \right)$$

8 Others

Stirling's formula

$$\ln(n!) = n \ln(n) - n + \frac{1}{2} \ln(2\pi n)$$

de Broglie relation

$$\epsilon = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

Energies

$$E_{kin} = \frac{1}{2} M \overline{v^2}$$
$$E_{rot} = \frac{1}{2} I \overline{\omega^2}$$