

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

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

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

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

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

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 $\times 2$

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

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

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

$$= \left(\sum_{j_1} e^{-\beta \epsilon_{1j_1}} \right) \dots \left(\sum_{j_N} e^{-\beta \epsilon_{Nj_1}} \right)$$

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

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

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

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:

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

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

Rotational modes

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

$$I = \mu r_0^2 \quad T_{rot} = \frac{\hbar^2}{Ik_B}$$

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

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:

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

partition sum:

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

$$\begin{aligned} \rightarrow Z &= \prod_{modes} z(\omega) \\ \rightarrow E &= -\partial_\beta \ln(Z) = \sum_{modes} \hbar\omega \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right) \\ &= E_0 + 3N \int_0^{\omega_D} d\omega \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \frac{3\omega^2}{\omega_D^3} \\ c_v(T) &= \frac{\partial E}{\partial T} \\ &= \frac{3\hbar^2 N}{k_B T^2} \int_0^{\omega_D} d\omega \frac{3\omega^2}{\omega_D^3} \frac{e^{\beta\hbar\omega} \omega^2}{\left(e^{\beta\hbar\omega} - 1\right)^2} \\ u &= \beta\hbar\omega \\ c_v(T) &= \frac{9Nk_B}{u_m^3} \int_0^{u_m} \frac{e^u u^4}{(e^u - 1)^2} du \end{aligned}$$

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

$$\begin{aligned} E &= \frac{4\sigma}{c} VT^4, \quad \sigma = \frac{\pi^2 k_B^4}{60\hbar^3 c^2} \\ c_v &= \frac{16\sigma}{c} VT^3 \end{aligned}$$

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

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:
 $\hbar\omega_{max} = 2.82k_B T$ Wien’s displacement law

4 The grandcanonical ensemble

$T, \mu = const.$

$$\begin{aligned} p_N(q,p) &= \frac{1}{\Xi_\mu(T,V)} e^{-\beta(H_N(q,p) - \mu N)} \\ \Xi_\mu(T,V) &= \sum_{N=0}^{\infty} \frac{1}{h^{3N} N!} \iint d^{3N}q d^{3N}p e^{-\beta(H_N - \mu N)} \\ \rightarrow \Xi_z &= \sum_{N=0}^{\infty} z^N Z_N(T,V) \end{aligned}$$

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

Mean phase space observable

$$\begin{aligned} \langle F \rangle &= \frac{1}{\Xi_\mu(T,V)} \sum_{N=0}^{\infty} \frac{1}{h^{3N} N!} \iint d^{3N}q d^{3N}p \dots \\ &\dots e^{-\beta(H_N - \mu N)} F_N(q,p) \end{aligned}$$

mean particle number:

$$\begin{aligned} \langle N \rangle &= \frac{1}{\beta} \left(\frac{\partial}{\partial \mu} \ln(\Xi_\mu(T,V)) \right)_{T,V} \\ &= z \left(\frac{\partial}{\partial z} \ln(\Xi_z(T,V)) \right)_{T,V} \end{aligned}$$

pressure:

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

energy U :

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

Grandcanonical potential

grandcanonical potential:

$$\begin{aligned} \Psi(T,V,\mu) &= -k_B T \ln(\Xi_\mu(T,V)) \\ p \text{ is maximal, if } \Psi \text{ is minimal.} \\ \text{Total differential:} \end{aligned}$$

$$\begin{aligned} d\Psi &= -SdT - pdV - \langle N \rangle d\mu \\ \text{Equations of state:} \\ S &= -\frac{\partial \Psi}{\partial T}, p = -\frac{\partial \Psi}{\partial V}, N = -\frac{\partial \Psi}{\partial \mu} \end{aligned}$$

Fluctuations

$$\begin{aligned} \sigma_N^2 &= \langle N^2 \rangle - \langle N \rangle^2 = \frac{1}{\beta^2} \left(\partial_\mu^2 \ln(\Xi_\mu) \right) \\ \frac{\sigma_N}{\langle N \rangle} &\propto \frac{1}{\sqrt{N}} \end{aligned}$$

Ideal gas

$$\begin{aligned} Z_N(T,V) &= \frac{1}{N!} \left(\frac{V}{\lambda^3} \right)^N, \quad \lambda = \frac{h}{(2\pi m k_B T)^{\frac{1}{2}}} \\ \Xi &= \sum_{N=0}^{\infty} Z_N(T,V) z^N \\ &= \sum_{N=0}^{\infty} \frac{1}{N!} \left(e^{\beta\mu} \frac{V}{\lambda^3} \right)^N \\ &= e^{z \frac{V}{\lambda^3}} \quad \text{fugacity: } z := e^{\beta\mu} \\ \langle N \rangle &= \frac{1}{\beta} \partial_\mu \ln(Z_G) = \frac{V}{\lambda^3} d^{\beta\mu} \\ \mu &= k_B T \ln \left(\frac{N \lambda^3}{V} \right) \end{aligned}$$

Molecular adsorption onto a surface

$$\begin{aligned} Z_G &= z_G^N; z_G = 1 + e^{-\beta(\epsilon - \mu)} \\ \langle n \rangle &= \frac{1}{e^{-\beta(\mu - \epsilon)} + 1} \quad \text{per site} \\ \langle \epsilon \rangle &= \epsilon \langle n \rangle \end{aligned}$$

5 Quantum fluids
Fermion vs. bosons
 Particles with half-integer (integer) spin are called fermions (bosons). Their total wave function (space and spin) must be antisymmetric (symmetric) under the exchange of any pair of identical particles.
Canonical ensemble
 two particles that are distributed over two states with energies 0 and ϵ

$$\begin{aligned} Z_F &= e^{-\beta\epsilon} \quad \text{Fermi-Dirac} \\ Z_B &= 1 + e^{-\beta\epsilon} + e^{-2\beta\epsilon} \quad \text{Bose-Einstein} \\ Z_M &= \frac{1 + 2e^{-\beta\epsilon} + e^{-2\beta\epsilon}}{2} \quad \text{Maxwell-Boltzmann} \end{aligned}$$

Grand canonical ensemble
 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:

$$\begin{aligned} n_F &= \Theta(\mu - \epsilon) \\ \text{Bosons:} \\ z_B &= \frac{1}{1 - e^{-\beta(\epsilon - \mu)}} \end{aligned}$$

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

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

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

$$\begin{aligned} \mu &= \epsilon_F \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{\epsilon_F} \right)^2 \right] \text{ for } T \ll \frac{\epsilon_F}{k_B} \\ c_V &= \frac{\partial E}{\partial T} \Big|_V = N \frac{\pi^2}{3} k_B^2 D(\epsilon_F) T \\ c_V &= N \frac{\pi^2}{2} \frac{k_B T}{\epsilon_F} k_B \end{aligned}$$

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.

$$\begin{aligned} N &= \frac{N}{\lambda^3} g_{\frac{3}{2}}(z) \\ z = e^{\beta\mu}, \quad \lambda &= \frac{h}{(2\pi m k_B T)^{\frac{1}{2}}} \end{aligned}$$

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

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

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

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

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

$$\begin{aligned} n_{F/B} &= \frac{1}{e^{\beta(\epsilon - \mu)} \pm 1} \rightarrow e^{\beta\mu} e^{-\beta\epsilon} \\ N &= g \frac{V}{\lambda^3} e^{\beta\mu} \\ E &= \frac{3}{2} k_B T N \end{aligned}$$

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:
 $\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{J}_i \vec{J}_j - \mu \vec{B} \sum_i \vec{J}_i$
 lattice gases:
 $\mathcal{H} = - \sum_{\langle i,j \rangle} J_{ij} S_i S_j$

1. Dimensional

Only Next Neighbor and $B_0 = 0$
 $J_{i,i+1} \rightarrow J_i, \quad \mathcal{H} = - \sum_{i=1}^{N-1} J_i S_i S_{i+1}, \quad J_i = \beta J_i$

$$\begin{aligned} Z_N &= \sum_{S_1} \dots \sum_{S_N} \exp \left(\sum_{i=1}^{N-1} J_i S_i S_{i+1} \right) \\ &= 2^N \prod_{i=1}^{N-1} \cosh(\beta J_i) \end{aligned}$$

Spin correlation function:

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

spontaneous magnetisation:

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

No phase transition for $T > 0$. But for $T = 0$
 $M_S(T=0) = \mu$

Transfer matrix

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

$$\begin{aligned} T_{i,i+1} &= e^{j S_i S_{i+1} + \frac{1}{2} b (S_i + S_{i+1})} \\ \rightarrow e^{-\beta \mathcal{H}} &= T_{1,2} \cdot T_{2,3} \dots T_{N,1} \\ T &= \begin{pmatrix} T(+1,+1) & T(+1,-1) \\ T(-1,+1) & T(-1,-1) \end{pmatrix} \\ Z_N &= \lambda_1^N + \lambda_2^N = E_+^N + E_-^N \end{aligned}$$

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

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