Theoretical Statistical Physics (MKTP1) Version: 23.3.2021

1 Introduction to probability theory Baves' 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

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

$$\mu = \langle i \rangle = \sum_{i} ip_{i} \text{ or } \mu = \langle x \rangle = \int xp(x)dx$$

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

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

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

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

Information entropy

$$S = -\sum_{i} p_{i} \ln(p_{i})$$

2 The microcanonical ensemble

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

The fundamental postulate

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

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

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

 n_0 different particles

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

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 excannge

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

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

$$dE = TdS - pdV + \mu dN$$

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 $\hat{H}(S, p, N) = U + pV$ G(T, p, N) = U + pV - TS

Ideal Gas

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

microcanonical partition sum for an ideal gas

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

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

Equations of state fo ideal gas

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

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

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

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

Einstein model for specific heat of a solid
$$E = \hbar \omega \left(\frac{N}{2} + Q \right) \rightarrow Q = \left(\frac{E}{\hbar \omega} - \frac{N}{2} \right)$$

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

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

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

$$e = E/E_0 ; E_0 = N\hbar\omega$$

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

Entropic elasticity of polymers

 $\begin{aligned} N_{+} - N_{-} &= \frac{L}{a} = m \to N_{+} = \frac{1}{2} \left(N + m \right) \\ \Omega &= \frac{N!}{N_{+}! N_{-}!} = \frac{N!}{\left(\frac{1}{2} \left(N + m \right) \right)! \left(\frac{1}{2} \left(N - m \right) \right)!} \end{aligned}$

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 $T_1 = T_2$

$$S_{i} = \frac{3}{2}k_{B}N_{i}\ln(E_{i}) + \text{independent of } E_{i}$$

$$S = S_{1} + S_{2}$$

$$dS = 0 \rightarrow \frac{\partial S_{1}}{\partial E_{1}} = \frac{\partial S_{2}}{\partial E_{2}}$$

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

consider small deviation:

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

$$S(\overline{E}_1 + \Delta E) \approx \frac{3}{2} k_B \left[N_1 \ln \overline{E}_1 + N_2 \ln \overline{E}_2 - \frac{N_1}{2} \left(\frac{\Delta E}{\overline{E}_1} \right)^2 - \frac{N_2}{2} \left(\frac{\Delta E}{\overline{E}_2} \right)^2 \right]$$

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

3 The canonical ensemble

T = const, V = const, N = const. **Boltzmann distribution**

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

For classical Hamiltonian systems:

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

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

total differential:

equations of state

Non-interacting systems

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

 $Z = \sum_{i_1} \sum_{i_2} \dots \sum_{i_{N}} e^{-\beta \sum_{i=1}^{N} \epsilon_{ij_i}}$

 $=z_1\cdot\dots\cdot z_N=\prod^N z_i$

TODO: ADD EXAMPLES

Equipartition theorem

f are the degrees of freedom.

harmonic Hamiltonian with f = 2

 $\mathcal{H} = Aa^2 + Bp^2$

 $\propto \left(T^{\frac{1}{2}}\right)^{3}$

sum ('equipartition theorem')

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

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

For sufficiently high temperture (classical limit), each quadratic term in the Hamilto-

nian contributes a factor $T^{\frac{1}{2}}$ to the partition

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

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

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

 $c_v = \frac{dU}{dT} = \frac{f}{2}k_B$

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

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

 $= \left(\sum_{i,j} e^{-\beta \epsilon_1 j_1} \right) \dots \left(\sum_{i,j} e^{-\beta \epsilon_N j_1 N} \right)$

 $dF = dE + d(TS) = -SdT - pdV + \mu N$

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

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

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

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

$$Z_x = z_x^N$$

Vibrational modes

Molecular gases

often described by the Morse potential:

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

An exact solution of the Schrödinger equation

$$\begin{split} E_n &= \hbar \omega_0 \left(n + \frac{1}{2} \right) - \frac{\hbar^2 \omega_0^2}{e E_0} \left(n + \frac{1}{2} \right)^2 \\ \omega_0 &= \frac{\alpha}{2\pi} \sqrt{\frac{2E_0}{\mu}}, \quad \mu = \frac{m}{2} \end{split}$$

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

$$\begin{split} z_{vib} &= \frac{e^{-\beta\hbar\omega/2}}{1 - e^{-\beta\hbar\omega_0}} \\ T_{vib} &\approx \frac{\hbar\omega_0}{k_B} \approx 6.140 K \ \text{for} \ H_2 \end{split}$$

Rotational modes

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

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

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

Nuclear contributions: ortho- and parahydro-

$$z_{ortho} = \sum_{l=1,3,5,...} (2l+1)e^{-\frac{l(l+1)T_{rot}}{T}}$$
$$z_{para} = \sum_{l=0,2,4} (2l+1)e^{-\frac{l(l+1)T_{rot}}{T}}$$

Theoretical Statistical Physics (MKTP1) Version: 23.3.2021

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:

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

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

density of states in ω -space:

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

count modes in frequency-space:

$$\sum_{modes}(\dots) = 3\sum_{k}(\dots) = 3N\int_{0}^{\omega_{D}}d\omega D(\omega)(\dots)$$

partition sum:

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

$$\begin{split} & \to Z = \prod_{modes} z(\omega) \\ & \to E = -\partial_\beta \ln(Z) = \sum_{modes} \hbar \omega \left(\frac{1}{e^{\beta \hbar \omega} - 1} + \frac{1}{2} \right) \\ & = E_0 + 3N \int_0^{\omega_D} d\omega \frac{\hbar \omega}{e^{\beta \hbar \omega} - 1} \frac{3\omega^2}{\omega_D^3} \\ & c_v(T) = \frac{\partial E}{\partial T} \end{split}$$

$$c_v(T) = \frac{1}{\partial T}$$

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

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

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

$$c_v(T) = 3Nk_B$$

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

$$c_{\nu}(T) = \frac{12\pi^4}{5} N k_B \left(\frac{T}{T_D}\right)^3$$

Black body radiation

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

$$J = \frac{P}{A} = \sigma T^4$$
 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:

 $\hbar\omega_{max} = 2.82k_BT$ Wien's displacement law

4 The grandcanonical ensemble **Probability distribution**

T and μ are fixed.

$$p_i = \frac{1}{Z_G} e^{-\beta(E_i - \mu N_i)} \text{ prob. distribution}$$

$$Z_G = \sum_i e^{-\beta(E_i - \mu N_i)} \text{ partition sum}$$

$$\Psi = -k_B T \ln(Z_G) \text{ grandcanonical pot.}$$

Grandcanonical potential

The probability to have a macroscopic value (E,N) is:

$$p(E,N) = \frac{1}{Z_G} \Omega(E,N) e^{-\beta(E-\mu N)}$$
 two particles that are C states with energies 0 an
$$= \frac{1}{Z_G} e^{-\beta(E-TS-\mu N)} = \frac{1}{Z_G} e^{-\beta\Psi(T,V,\mu)}$$
 $Z_F = e^{-\beta\varepsilon}$ Fermi-Dirac

grandcanonical potential:

$$\Psi(T, V, \mu) := E - TS - \mu N$$

p is maximal, if Ψ is minimal. Total differential:

$$\begin{split} d\Psi &= d(E - TS - \mu N) \\ &= TdS - pdV + \mu dN - d(TS + \mu N) \\ &= -SdT - pdV - Nd\mu \end{split}$$

Equations of state:

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

Fluctuations

$$\langle N \rangle = \sum_{i} p_{i} N_{i} = \frac{1}{\beta} \partial_{\mu} \ln(Z_{G})$$

$$\sigma_{N}^{2} = \langle N^{2} \rangle - \langle N \rangle^{2} = \frac{1}{\beta^{2}} \partial_{\mu}^{2} \ln(Z_{G})$$

$$\frac{\sigma_{N}}{\langle N \rangle} \propto \frac{1}{N^{\frac{1}{2}}}$$

Ideal gas

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

Molecular adsorption onto a surface

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

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

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

$$Z_F = e^{-\beta \epsilon}$$
 Fermi-Dirac

$$Z_B = 1 + e^{-\beta \epsilon} + e^{-2\beta \epsilon}$$
 Bose-Einstein

$$Z_M = \frac{1 + 2e^{-\beta\epsilon} + e^{-2\beta\epsilon}}{2}$$
 Maxwell-Boltzmann

Grand canonical ensemble

Fermions:

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

average occupation number n_F :

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

For $T \to 0$, 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:

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

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

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

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

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

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

_Fermi pressure

$$p \stackrel{T \to 0}{\to} \frac{2}{5} \frac{N}{V} \epsilon_F = \frac{(2\pi^2)^{\frac{2}{3}}}{5} \frac{\hbar^2}{mv^{\frac{5}{3}}}$$

The ideal Bose fluid

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

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

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

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

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

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

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

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:

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

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

1. Dimensional

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

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

Spin correlation function:

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

spontanious magnetisation:

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

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

Transfer matrix

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

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

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

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

Renormalization of the Ising chain

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

Renormalization of the 2d Ising model

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

Theoretical Statistical Physics (MKTP1) Version: 23.3.2021

The 2d Ising model

$$\beta \mathcal{H} = -K \sum_{r,c} S_{r,c} S_{r+1,c} - K \sum_{r,c} S_{r,c} S_{r,c+1}$$

$$1 = \sinh(2K_c)$$

$$K_c = \frac{1}{2} \ln\left(1 + \sqrt{2}\right) \approx 0.4407$$

$$T_c = 2J/\ln\left(1 + \sqrt{2}\right) \approx 2.269J/k_B$$

Perturbation theory

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

Mean field theory for the Ising model

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

$$\mathcal{H}_0 = -B \sum_i S_i$$

$$F_0 = -Nk_B T \ln(e^{\beta B} + e^{-\beta B})$$

$$= -Nk_B T \ln(2\cosh(\beta B))$$

$$F \le F_0 + \langle \mathcal{H} - \mathcal{H}_0 \rangle_0$$

$$= -Nk_B T \ln(2\cosh(\beta B)) - N\frac{z}{2} \langle S \rangle_0^2$$

$$+ N\langle S \rangle_0 = F_u$$

$$\rightarrow z = 2 \cdot \text{dimension}$$

$$B = Jz \langle S \rangle_0 = Jz \tanh(\beta B)$$

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

7 Classical fluids

Virial expansion

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

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

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