Lattice Gas

(d-dimension)

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

$$Q_N(T,V) = \int d^{dN}x \, e^{-\beta U(\bar{x}_1, \bar{x}_2, \dots, \bar{x}_N)}$$

$$U(\bar{x}_1, \bar{x}_2, \dots, \bar{x}_N) = \sum_{i<j} U(\bar{x}_i - \bar{x}_j) \qquad \text{tr. inv. (hom.) system}$$

$$\rho(\bar{x}) = \sum_{i=1}^{N} \delta(\bar{x} - \bar{x}_i) \qquad \text{(density)}$$

$$\sum_{i<j} U(\bar{x}_i - \bar{x}_j) = \frac{1}{2} \sum_{i \neq j} U(\bar{x}_i - \bar{x}_j) = \frac{1}{2} \sum_{i \neq j} \iint U(\bar{x} - \bar{x}') \delta(\bar{x} - \bar{x}_i) \delta(\bar{x}' - \bar{x}_j) \, d^dx \, d^dx'$$

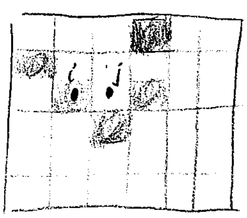
$$= \frac{1}{2} \iint d^dx \, d^dx' \, U(\bar{x} - \bar{x}') \left[\sum_{i,j} \delta(\bar{x} - \bar{x}_i) \delta(\bar{x}' - \bar{x}_j) - \sum_i \delta(\bar{x} - \bar{x}_i) \delta(\bar{x}' - \bar{x}_i) \right]$$

$$= \frac{1}{2} \iint d^dx \, d^dx' \, U(\bar{x} - \bar{x}') \left[\rho(\bar{x}) \rho(\bar{x}') - \delta(\bar{x} - \bar{x}') \rho(\bar{x}) \right]$$

first term: $\frac{1}{2} \iint d^dx \, d^dx' \, U(\bar{x} - \bar{x}') \rho(\bar{x}) \rho(\bar{x}') \Longrightarrow \frac{1}{2} \sum_{i,j} U_{ij} n_i n_j =$

second term: $-\frac{1}{2} U(0) \underbrace{\int \rho(\bar{x}) d^dx}_{N} = -\frac{1}{2} U(0) N$

U_{ij}



\# of sites

$\downarrow$

$\mathcal{N} = \mathcal{L}^d$

$L = \mathcal{L} a$

$V = L^d$

$(n_i^2 = n_i)$

$U_{ij} = U(i-j)$

$$n_i = \begin{cases} 0 & \text{empty} \\ 1 & \text{occupied} \end{cases}$$

$$N = \sum_{i=1}^{\mathcal{N}} n_i$$

$$\frac{n_i}{a^d} \to \rho(\bar{x})$$

$$\frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{2} \sum_i U_{ii} n_i^2 = \frac{1}{2} \sum_{i \neq j} U_{ij} n_i n_j + \frac{1}{2} U(0) \underbrace{\sum_i n_i}_{N}$$

"lattice" constant a: ~ related to hard core $\qquad \sum_{i=1}^{\mathcal{N}} n_i = N$

$$\int d^d x_1\, d^d x_2 \dots d^d x_N (\dots) \longrightarrow (a^d)^N N! \sum_{n_1, n_2, \dots n_{\mathcal{N}}}{}' (\dots) = a^{Nd} N! \sum_{\{n_k\}}{}' (\dots)$$

$$Q_N(T,V) = a^{Nd}\, N! \sum_{\{n_k\}}{}' e^{-\beta \frac{1}{2}\sum_{i \neq j} U_{ij} n_i n_j}$$

$$Z_G = \sum_{N=0}^{\infty} \frac{1}{\cancel{N!}} \left(\frac{e^{\beta\mu}}{\lambda^d}\right)^N a^{Nd}\, \cancel{N!} \sum_{\{n_k\}}{}' e^{-\beta \frac{1}{2}\sum_{i \neq j} U_{ij} n_i n_j}$$

$$= \sum_{\{n_k\}} \left(e^{\beta\mu} \frac{a^d}{\lambda^d}\right)^N e^{-\beta \frac{1}{2}\sum_{i\neq j} U_{ij} n_i n_j} = \qquad N = \sum_{i=1}^{\mathcal{N}} n_i$$

$$= \sum_{\{n_k\}} e^{[\beta\mu + d \ln a/\lambda] \sum_{i=1}^{\mathcal{N}} n_i}\; e^{-\beta \frac{1}{2}\sum_{i\neq j} U_{ij} n_i n_j}$$

$$= \sum_{\{n_k\}} e^{-\beta\left[\frac{1}{2}\sum_{i\neq j} U_{ij} n_i n_j - \left(\mu + \frac{d}{\beta}\ln(a/\lambda)\right)\sum_i n_i\right]}$$

$U(\bar{x}_i - \bar{x}_j)$ is short ranged $\Rightarrow$ keep only "~~nearest~~-neighbor" interaction terms.

$$U_{ij} = \begin{cases} U & \text{if } i,j \text{ are n.n. neighbors} \\ 0 & \text{otherwise} \end{cases}$$

$$\mathcal{H}\{n_k\} = U \sum_{\langle ij \rangle} n_i n_j - \qquad \bar{\mu} \equiv \mu + \frac{d}{\beta}\ln(a/\lambda)$$

lattice $\qquad$ physical

$$Z_G \simeq Z_{\text{lattice gas}} = \sum_{\{n_k\}} e^{-\beta\left(\mathcal{H}\{n_k\} - \bar{\mu}\sum_{i=1}^{N} n_i\right)}$$

lattice gas:

$$Z_{\text{lattice gas}} = \sum_{\{n_k\}} e^{-\beta\left[U\sum_{\langle ij\rangle} n_i n_k - \bar{\mu}\sum_i n_i\right]} \qquad n_i = \begin{cases} 0 & \text{empty} \\ 1 & \text{occupied}\end{cases}$$

The Ising Model

from the quantum mechanical exchange interaction:

$$\mathcal{H} = -J_0 \sum_{\langle ij\rangle} \bar{S}_i \cdot \bar{S}_j$$ Heisenberg model

$\uparrow$ exchange interaction energy

Ising model:

N: # of lattice sites

$$\mathcal{H} = -J_0 \sum_{\langle ij\rangle} S_i^z S_j^z$$

reasonable for highly anisotropic thin film ferromagnets

$\bar{e}$; $\quad S_i^z = \pm\frac{\hbar}{2} \qquad i = 1, 2, \ldots, N$

with external field $H \# \hat{z}$

$$\boxed{\mathcal{H}_{\text{Ising}} = -J \sum_{\langle ij\rangle} s_i s_j - H\sum_i s_i}$$

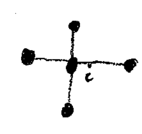
$J > 0$ ferromagnet

$s_i = \pm 1$

Phase Transition: $\quad T \to 0 \quad$ ground state $\quad s_i = \pm 1 \;\; \forall i$

$\boxed{H = 0}$

$$E_0 = -\frac{1}{2} J N q$$



q: # of nearest neighbors

$F = E - TS \qquad T \to \infty \quad$ entropy dominates, system disordered

is there a T_c, such that

$$m = \langle S_i\rangle = \begin{cases} 0 & T \geq T_c \\ \neq 0 & T < T_c \end{cases}$$ order parameter

Equivalence of the Lattice gas and the Ising model

Ising $\quad S_i = \pm 1$

Lattice Gas $\quad n_i = \pm 1$

$\bar{\mu} \to \mu$ for simplicity

$$\mathcal{H}_{Ising} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i$$

$$\mathcal{H}_{latt} - \mu N = U \sum_{\langle ij \rangle} n_i n_j - \mu \sum_{i=1}^{\mathcal{N}} n_i$$

$$\begin{array}{ccc} S_i & & n_i \\ -1 & \leftrightarrow & 0 \\ +1 & \leftrightarrow & 1 \end{array}$$

$$\boxed{n_i = \frac{1}{2}(1 + S_i)}$$

$\mathcal{N}$ lattice sites

$$\left(\left\langle \frac{n_i}{a^d} \right\rangle = \frac{N}{V} \right)$$

$$\mathcal{H}_{lattice} - \mu N = U \sum_{\langle ij \rangle} \frac{1}{4}(1+S_i)(1+S_j) - \mu \sum_i \frac{1}{2}(1+S_i)$$

$$= U \sum_{\langle ij \rangle} \frac{1}{4}[1 + S_i + S_j + S_i S_j] - \mu \frac{1}{2} \sum_i 1 - \frac{\mu}{2} \sum_i S_i$$

$$= \frac{1}{8} U \mathcal{N} q + \frac{1}{4} U q \sum_i S_i + \frac{U}{4} \sum_{\langle ij \rangle} S_i S_j - \frac{1}{2} \mu \mathcal{N} - \frac{\mu}{2} \sum_i S_i$$

$$= \frac{1}{8} U \mathcal{N} q - \frac{1}{2} \mu \mathcal{N} + \frac{U}{4} \sum_{\langle ij \rangle} S_i S_j - \left(\frac{\mu}{2} - \frac{U}{4} q \right) \sum_{i=1}^{\mathcal{N}} S_i$$

$$= E_0 - J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i = E_0 + \mathcal{H}_{Ising}$$

$$\boxed{\begin{aligned} J &= -\frac{U}{4} \\ H &= \frac{\mu}{2} - \frac{Uq}{4} \end{aligned}}$$

exact mapping between the Ising model and the lattice-gas

q: # of nearest neighbors ($q = 2d$ on regular lattice)

$$Z_{lattice\ gas}(T, \mu, \mathcal{N}) = e^{-\beta E_0} Z_{Ising}(T, H, \mathcal{N})$$

$\mathcal{N}$ sites

The Ising model

$$\mathcal{H} = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_i S_i$$

$S_i = \pm 1$

$J > 0$ (ferromagnet)

N lattice sites

at each site we can represent $S_i = \pm$ magn. moment.

$\uparrow\uparrow \quad \downarrow\downarrow \quad E_J = -J$

$\downarrow\uparrow \quad \uparrow\downarrow \quad E_J = +J$

Phase transition - Spontaneous Symmetry Breaking

$H = 0$ (no external field)

order parameter : $m = \left\langle \frac{1}{N} \sum_{i=1}^{N} S_i \right\rangle$ (magnetization)

tr. invariance: $m = \frac{1}{N} N \langle S_i \rangle = \langle S_i \rangle \quad \forall\, i = 1, 2, \ldots, N$

motivation: high temperature: $P[\{S_i\}] = \dfrac{e^{-\frac{\mathcal{H}[\{S_i\}]}{kT}}}{Z}$

$$Z_N(T, H) = \sum_{\{S_i\}} e^{\frac{\mathcal{H}[\{S_i\}]}{kT}}$$

$T \to \infty \quad P[\{S_i\}] = \text{const.}$

(entropy wins) disordered phase $\langle S_i \rangle = 0 \quad \boxed{m = 0}$

low temperature : $T \to 0$ (ground state)

$E_0 = -\frac{1}{2} J N q$ coordination number

$\langle S_i \rangle = +1 \quad \forall i$

or

$\langle S_i \rangle = -1$ (double degeneracy)

ordered phase $m = +1$ (or -1)

Weiss mean-field theory (molecular field approx.)

$\hbar$, etc. scaled into H

$$\mathcal{H} = -J\sum_{\langle ij\rangle} S_i S_j - H\sum_i S_i \qquad \langle S_i\rangle = m$$

$$S_i = \langle S_i\rangle + (S_i - \langle S_i\rangle) = m + (S_i - m)$$

$$\mathcal{H} = -J\sum_{\langle ij\rangle}[m + (S_i - m)][m + (S_j - m)] - H\sum_i S_i$$

fluctuations: neglect

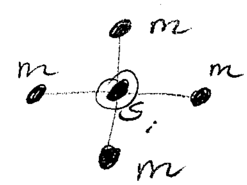
$$= -J\sum_{\langle ij\rangle} m^2 - Jm\sum_{\langle ij\rangle}(S_i - m) - Jm\sum_{\langle ij\rangle}(S_j - m) - \overbrace{J\sum_{\langle ij\rangle}(S_i - m)(S_j - m)} - H\sum_i S_i =$$

note: $S_i S_j = [m + (S_i - m)][m + (S_j - m)] = m^2 + m(S_i - m) + m(S_j - m) + (S_i - m)(S_j - m)$
$= m^2 + mS_i - m^2 + mS_j - m^2 + (S_i - m)(S_j - m) \approx -m^2 + mS_i + mS_j$ ← mean field

$$\cong +\frac{1}{2}Jm^2Nq - Jmq\sum_i S_i - H\sum_i S_i$$

$$= \frac{1}{2}Jm^2Nq - \underbrace{(Jmq + H)}_{\text{effective molecular field}}\sum_i S_i$$

Weiss (1907)



$$Z_N(T,H) = \sum_{S_1,S_2,\ldots,S_N} e^{-\beta\mathcal{H}[\{S_i\}]} = e^{-\beta\frac{1}{2}Jm^2Nq}\left[\sum_{S_i=\pm 1} e^{\beta(Jmq+H)S_i}\right]^N$$

$$= e^{-\beta\frac{1}{2}Jm^2Nq}\left[2\cosh\left(\beta(Jmq + H)\right)\right]^N = \left[e^{-\beta\frac{J}{2}m^2q}\, e^{\ln 2 + \ln\cosh(\;)}\right]^N$$

self-consistency: ($m = ?$)

$$m = \langle S_i\rangle = \frac{1}{N}\left\langle\sum_i S_i\right\rangle = \frac{1}{N}\frac{\partial}{\partial(\beta H)}\ln Z_N(T,H)$$

$$\downarrow$$

$$\frac{1}{\beta}\frac{\partial}{\partial H}$$

$$m = \frac{1}{N}\frac{1}{\beta}\frac{\partial}{\partial H}\left\{-\frac{\beta}{2} J m^2 q N + N \ln 2 + N \ln \cosh\left[\beta (J m q + H)\right]\right\}$$

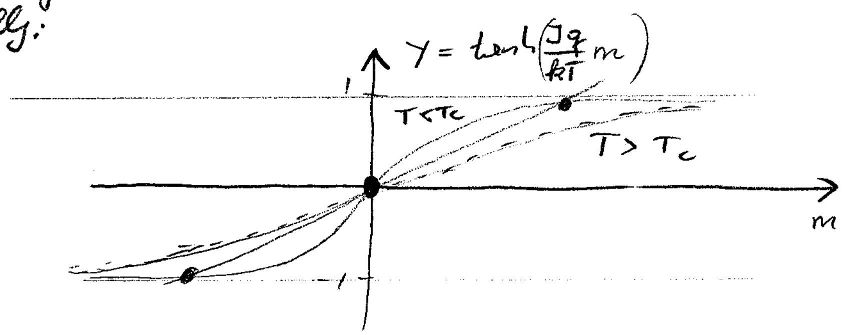
$$= \frac{1}{\beta}\frac{\partial}{\partial H} \ln \cosh\left[\beta J m q + \beta H\right] = \tanh\left(\beta J m q + \beta H\right)$$

$$\boxed{m = \tanh(\beta J q m + \beta H)}$$

for the spontaneous magnetisation: $H = 0$

obtain solution graphically:

$$\boxed{m = \tanh\left(\frac{Jq}{kT} m\right)}$$



slope of $\tanh(x)$ at $x = 0$:

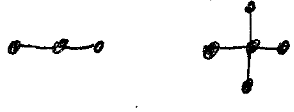
$$\boxed{\tanh(x) = x - \frac{x^3}{3} + \frac{2x^5}{15} \pm \ldots}$$

$\tanh'(x) = 1$ at $x = 0$

$m \neq 0$ solution exist if $\frac{Jq}{kT} > 1$

i.e. $\frac{Jq}{kT_c} = 1$ $\boxed{kT_c = Jq = 2dJ}$

q: coordination number (number of nearest neighbors)



$q = 2d$ on regular hypercubic lattices in d dimension