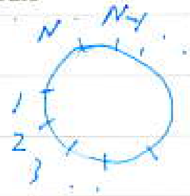
1D Ising chain exact solution

Date

$$E = -J\sum_{i=1}^{N}\sigma_i\sigma_{(i+1)\bmod N} - h\sum_{i=1}^{N}\sigma_i$$

$\therefore$ $N+1$ is same as 1



$$= -\sum_{i=1}^{N}\left(J\sigma_i\sigma_{i+1} + \frac{h}{2}(\sigma_i+\sigma_{i+1})\right) = -\sum_{i=1}^{N}E(\sigma_i,\sigma_{i+1})$$

$E(\sigma_i\,\sigma_{i+1}) =$
$J(\sigma_i\sigma_{i+1}) + \frac{h}{2}(\sigma_i+\sigma_{i+1})$

$$Z = \sum_{\sigma_1}\sum_{\sigma_2}\cdots\sum_{\sigma_N} e^{\sum_{i=1}^{N}\beta\left(J\sigma_i\sigma_{i+1} + \frac{h}{2}(\sigma_i+\sigma_{i+1})\right)}$$

$$= \sum_{\sigma_1}\sum_{\sigma_2}\sum_{\sigma_3}\cdots\sum_{\sigma_N} e^{\beta E(\sigma_1\sigma_2)}\, e^{\beta E(\sigma_2\sigma_3)}\, e^{\beta E(\sigma_3\sigma_4)}\cdots e^{\beta E(\sigma_N\sigma_1)}$$

define $P(\sigma_i\,\sigma_{i+1}) = e^{\beta E(\sigma_i\,\sigma_{i+1})} = P_{\sigma_i,\sigma_{i+1}}$

$$P = \begin{array}{c|cc} & \sigma_{i+1}=+1 & \sigma_{i+1}=-1 \\ \hline \sigma_i=+1 & e^{\beta(J+h)} & e^{-\beta J} \\ \sigma_i=-1 & e^{-\beta J} & e^{\beta(J-h)} \end{array}$$

$$(AB)_{ij} = \sum_k A_{ik}B_{kj}$$

$$= \sum_{\sigma_1\sigma_2\cdots\sigma_N} P_{\sigma_1\sigma_2}P_{\sigma_2\sigma_3}P_{\sigma_3\sigma_4}\cdots P_{\sigma_N\sigma_1}$$

$$= \mathrm{Tr}\,\underbrace{P\cdot P\cdots P}_{N} = \mathrm{Tr}\,P^N = \mathrm{Tr}\,SPS^{-1}SPS^{-1}SP\cdots P$$

$$= \mathrm{Tr}\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}^N$$

$$SPS^{-1} = \begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}$$

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

~~det~~

$$\det(P-\lambda I) = \det\begin{pmatrix} e^{\beta(J+h)}-\lambda & e^{-\beta J}\\ e^{-\beta J} & e^{\beta(J-h)}-\lambda\end{pmatrix} = 0$$

$$\det\begin{bmatrix} a\cdot b-\lambda & \frac{1}{a}\\ \frac{1}{a} & \frac{a}{b}-\lambda\end{bmatrix} = 0$$

Let $a = e^{\beta J}$
$b = e^{\beta h}$

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$$\sinh^2 x - \cosh^2 x = -1$$

$$\frac{e^{2x} - 2 + e^{-2x}}{4} - \frac{e^{2x} + 2 + e^{-x}}{4}$$

$$\frac{\cancel{e^{\beta J}}\sinh(\beta h) + \cancel{e^{\beta J}}\dfrac{\sinh(\beta h)\cosh(\beta h)}{\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}}{\cancel{e^{\beta J}}\cosh(\beta h) + \cancel{e^{\beta J}}\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}}$$

$$= \frac{\sinh(\beta h)\sqrt{\sinh^2(\beta h) + e^{-4\beta J}} + \sinh(\beta h)\cosh(\beta h)}{\cosh(\beta h)\sqrt{\sinh^2(\beta J) + e^{-4\beta J}} + \sinh^2(\beta h) + e^{-4\beta J}}$$

$$(a\cdot b-\lambda)\left(\frac{a}{b}-\lambda\right)-\left(\frac{1}{a}\right)^2=0$$

Date

$$a^2-\left(ab+\frac{a}{b}\right)\lambda+\lambda^2-\frac{1}{a^2}=0$$

$$\lambda^2-a\left(b+\frac{1}{b}\right)\lambda+a^2-\frac{1}{a^2}=0$$

$$\lambda_\pm=\frac{1}{2}\left(a\left(b+\frac{1}{b}\right)\pm\sqrt{a^2\left(b+\frac{1}{b}\right)^2-4\left(a^2-\frac{1}{a^2}\right)}\right)$$

$$=e^{\beta J}\left(\frac{e^{\beta h}+e^{-\beta h}}{2}\right)\pm\sqrt{e^{2\beta J}\left(\frac{e^{\beta h}+e^{-\beta h}}{2}\right)^2-\left(e^{2\beta J}-e^{-2\beta J}\right)}$$

$$=e^{\beta J}\cosh(\beta h)\pm\sqrt{e^{2\beta J}\underbrace{\cosh^2(\beta h)}_{\sinh^2(\beta h)+1}-e^{2\beta J}+e^{-2\beta J}}$$

$$=e^{\beta J}\cosh(\beta h)\pm\sqrt{e^{2\beta J}\sinh^2(\beta h)+e^{-2\beta J}}$$

$$\lambda_+>\lambda_-$$

$$F=-k_BT\ln\left(\lambda_1^N+\lambda_2^N\right)\qquad N\to\infty$$

$$=-k_BT\ln\lambda_1^N\left(1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right)$$

$$\left(\frac{\lambda_2}{\lambda_1}\right)^N\to 0 \text{ as } N\to\infty$$

$$=-Nk_BT\ln\lambda_1$$

magnetization

$$M=-\frac{\partial F}{\partial h}=-\frac{\partial}{\partial h}\left(-\frac{N}{\beta}\ln\lambda_1\right)$$

$$=N\frac{1}{\beta\lambda_1}\frac{\partial}{\partial h}\lambda_1=\frac{N\beta}{\beta\lambda_1}\left[e^{\beta J}\sinh(\beta h)+\frac{2e^{2\beta J}\sinh(\beta h)\cosh(\beta h)}{2\sqrt{e^{2\beta J}\sinh^2(\beta h)+e^{-2\beta J}}}\right]$$

$$=N\frac{\sinh\beta h}{\sqrt{\sinh^2(\beta h)+e^{-4\beta J}}}$$

$J=0$, we get

$$M=N\tanh(\beta h)$$

Date

$$e^{\beta J \sigma_i \sigma_{i+1}} = \cosh(\beta J) + \sigma_i \sigma_{i+1} \sinh(\beta J)$$

$$Z = \sum_{\{\sigma\}} \prod_{i=1}^{N} \cosh(\beta J) \left[1 + \sigma_i \sigma_{i+1} \tanh(\beta J) \right] \qquad \sigma^2 = 1$$

$$= \cosh^N(\beta J) \sum_{\{\sigma\}} \Big[1 + \underbrace{\sigma_1 \sigma_2 \cdot \sigma_2 \sigma_3 \cdots \sigma_{N-1} \sigma_N \sigma_N \sigma_1}_{1} \tanh^N(\beta J) \Big]$$

$$= 2^N \cosh^N(\beta J) \left(1 + \tanh^N(\beta J) \right)$$

$$\lambda_+ = e^{\beta J}\cosh(\beta h) + e^{\beta J}\sqrt{\sinh^2(\beta h) + e^{-4\beta J}}$$

$$\frac{\partial \ln \lambda_+}{\partial h} = \frac{1}{\lambda_+}\frac{\partial \lambda_+}{\partial h} = \frac{e^{\beta J}\left[\sinh(\beta h) + \frac{1}{\cancel{2}}\frac{\cancel{2}\sinh(\beta h)\cosh(\beta h)}{\sqrt{\sinh^2(\beta h)+e^{-4\beta J}}}\right]}{e^{\beta J}\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h) + e^{-4\beta J}}\right)}$$

$$= \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h)+e^{-4\beta J}}}\;\frac{\cancel{\sqrt{\sinh^2(\beta h)+e^{-4\beta J}} + \cosh(\beta h)}}{\cancel{\left(\cosh(\beta h) + \sqrt{\sinh^2(\beta h)+e^{-4\beta J}}\right)}}$$

$$= \frac{\sinh(\beta h)}{\sqrt{\sinh^2(\beta h)+e^{-4\beta J}}}$$

$\lim_{h\to 0} M \to 0$

$\lim_{h\to 0^+}\lim_{T\to 0} M = 1$

pair correlation function

$h = 0$ for simplicity

$$g(j) = \langle \sigma_0 \sigma_j \rangle = \langle \sigma_i \sigma_{i+j} \rangle$$

$$= \sum_{\{\sigma\}} \sigma_0 \sigma_j \, e^{\beta J(\sigma_0\sigma_1 + \sigma_1\sigma_2 + \cdots \sigma_{N-1}\sigma_0)} \frac{1}{Z}$$

$\tanh x = \frac{\sinh x}{\cosh x}$

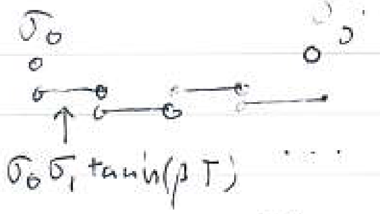
$$e^{\beta J \sigma_1\sigma_2} = \cosh(\beta J)\left[1 + \sigma_1\sigma_2 \tanh(\beta J)\right] \cancel{\frac{1}{Z}}$$

$$= \frac{\sum_{\{\sigma\}} \sigma_0\sigma_j \prod_{i=0}^{N-1}\left(1 + \sigma_i\sigma_{i+1}\tanh(\beta J)\right)}{\sum_{\{\sigma\}} \prod_{i=0}^{N-1}\left(1 + \sigma_i\sigma_{i+1}\tanh(\beta J)\right)}$$

$N \to \infty$

$$= \frac{1}{1}\left(\tanh^j(\beta J)\right)$$

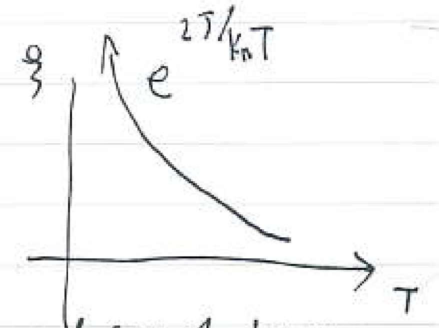
$$\left(\frac{\lambda_-}{\lambda_+}\right)^j$$



$$= e^{-\frac{j}{\xi}}$$

$$\tanh(\beta J) = e^{-\frac{1}{\xi}}$$

$$\xi = -\frac{1}{\ln\tanh(\beta J)} \underset{\beta\to\infty}{\approx} \frac{1}{2}e^{2\beta J}$$



typical size of domains

$+ + + + + - - - + - - -$

$\rightarrow \xi \leftarrow$

meaning of ξ

Date

1 (a) energy U.
volume V
particle number N

(b) Postulate II

(c) monotonicity $\frac{\partial S}{\partial U} \geq 0$

extensivity $S(\lambda U, \lambda V, \lambda N) = \lambda S(U, V, N)$

concavity $\frac{\partial^2 S}{\partial U^2} < 0$ or $2S(U) \geq S(U-\Delta U) + S(U+\Delta U)$

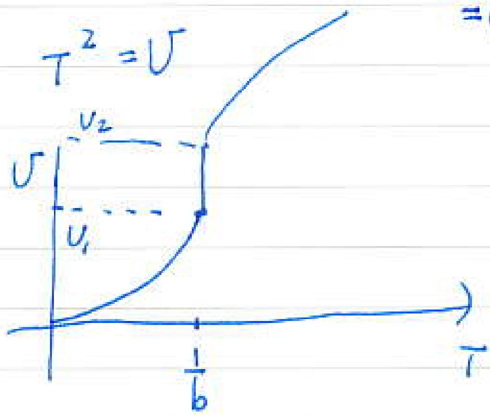
$S = 0$ when $T = \frac{\partial U}{\partial S} = 0$

2. (a)

(b) $$\frac{1}{T} = \frac{\partial S}{\partial U} = \begin{cases} \frac{1}{2} a \sqrt{\frac{N}{U}} & U < U_1 \\ b & U_1 \leq U \leq U_2 \\ \frac{1}{2} a' \sqrt{\frac{N}{U}} + d & U_2 < U \end{cases}$$

$$T = \begin{cases} \frac{2}{a} \sqrt{\frac{U}{N}} \\ \frac{1}{b} \\ \frac{1}{\frac{a'}{2}\sqrt{\frac{N}{U}} + d} \end{cases}$$

$\rightarrow$ $T^2 = U$



(c) $$\begin{cases} a\sqrt{U_1 N} = bU_1 + c \\ bU_2 + c = a'\sqrt{U_2 N} + dU_2 \\ \frac{1}{2} a \sqrt{\frac{N}{U_1}} = b \\ b = \frac{1}{2} a' \sqrt{\frac{N}{U_2}} + d \end{cases}$$

(d) $\Delta Q = T \Delta S$

$= \frac{1}{b}(S_2 - S_1)$

$= \frac{1}{b}(a'\sqrt{U_2 N} + dU_2 - a\sqrt{U_1 N})$

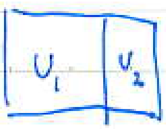
$= \frac{1}{b}(bU_2 + c - bU_1 - c)$

$= (U_2 - U_1)$

(e) $U = \lambda U_1 + (1-\lambda) U_2$

$S = \lambda S_1 + (1-\lambda) S_2$

$0 \leq \lambda \leq 1$



fraction

see C. Domb, "The Critical point" chap 14 K Huang

also J.M. Yeomans, or ~~Kubo, Toda, Hashitsume~~ Toda, Kubo, Saito

7 March 07

2D Ising model

$$E = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j \quad -h\sum\sigma_i$$

Date $h=0$

High-T expansion

$$Z = \sum_{\{\sigma\}} e^{\beta J \sum_{\langle ij\rangle}\sigma_i\sigma_j} = \sum_{\{\sigma\}}\prod_{\langle ij\rangle}\cosh K\cdot(1+\sigma_i\sigma_j\tanh K)$$

$K = \beta J = \frac{J}{k_B T}$

$$= \cosh^L K \sum_{\{\sigma\}}\prod(1+\sigma_i\sigma_j\tanh K)$$

L number of link.

$= \sum_{\langle ij\rangle} 1$

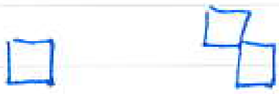
$$= 2^N\cosh^L K\left(1+\sum_{r=1}^{L} P(r)\tanh^r K\right)$$

from $\sum$

~~p(r) # of~~ polygons ~~that meets with an even # of~~ lines r

~~closed~~

~~for square lattice~~



but NOT

$P(r)$ the number of figures (graphs) with r lines composed of closed polygons (polygons can be disconnected). The lines must meet an even # of times at a site.

Low-T expansion

$$Z = \sum e^{\beta J\sum_{\langle ij\rangle}\sigma_i\sigma_j} = 2\cdot e^{K\cdot L}\left(1+\sum_{r=1}^{r_{max}} V(r)\, e^{-2rK}\right)$$

ground state degeneracy

r: number of + to − boundaries

V: number of configurations with r + to − boundaries

(Kramers & Wannier) 1941

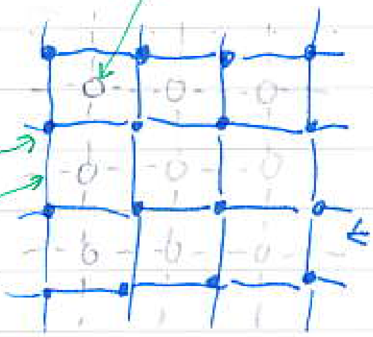
plaquette

Duality relation

① center of a plaquette is a dual site

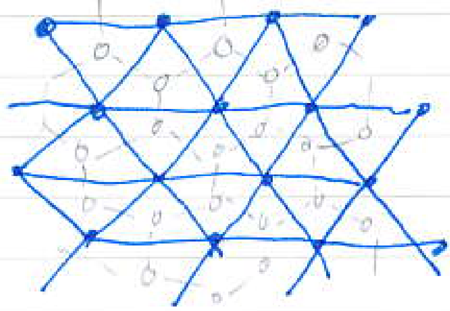
② dual line cross original line

square lattice



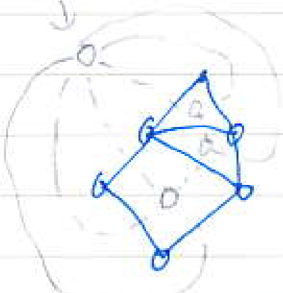
← ∞-large lattice

triangle lattice



the concept works for any planar graphs.

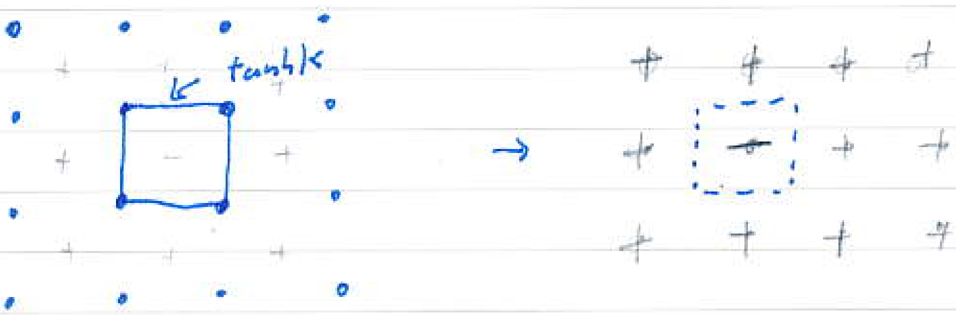
finite lattice



"The number of $P(r)$ for high-temperature expansion is exactly the same number of $V(r)$ in a low temperature expansion ~~at~~ on the dual lattice"

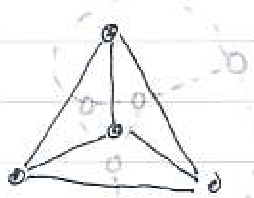
A configure (graph) for high-T expansion is also a config for Low-T expansion on dual lattice. The mapping is one-to-one.

original lattice → dual lattice



let use * to mean the same quantity in dual lattice

$$P(r) = \overset{*}{V}(r)$$
$$V(r) = P^*(r)$$



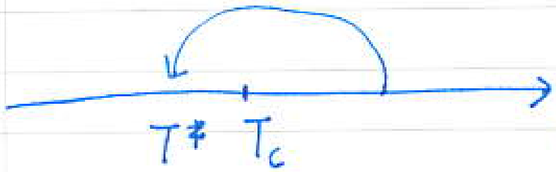
4-site self-dual finite lattice (graph or not)

$$Z(N,K) = 2^N (\cosh K)^L \left(\sum_{r=0}^{L} p(r) \tanh^r K \right)$$ partition fn at any lattice

$$Z^*(N^*, K^*) = 2 \exp(K^* L^*) \left(\sum_{r=0}^{r^*_{max}} p(r)\, e^{-2K^* r} \right)$$ Date $p(0) = 1$

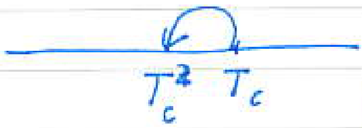
$$\frac{Z(N,K)}{2^N (\cosh K)^L} = \frac{Z^*(N^*, K^*)}{2 e^{K^* L^*}}$$ if we choose $\tanh K = e^{-2K^*}$

for square lattice $Z = Z^*$ because self-dual
$N = N^*$ $\left\{ \begin{matrix} L = L^* \\ N = N^* \end{matrix} \right.$



if $T_c \neq T_c^*$

at T_c f is singular in $N \to \infty$ then



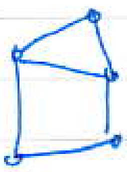
we would have 2 singular points (two phase transitions). but if we assume there is only one unique singular pt. then we must have $T_c = T_c^*$ or $\tanh K_c = e^{-2K_c}$

$K_c \approx 0.4407 = .44068679$ or $e^{-2K_c} = \sqrt{2} - 1$

symmetric for $\sinh(2K) \sinh(2K^*) = 1$

topological relation $L = L^*$
$N + N^* = L + 2$ Euler relation

# of site − # of lines + # of faces = 2



$N = 5$
$N^* = 3$
$L = 6$

$v - e + f = 2$

valid for planar graphs or simply connected polygons

3. $\mathcal{H} = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2$

(a) $Z = \frac{1}{h} \int dp \int dq \; e^{-\beta\left(\frac{p^2}{2m} + \frac{1}{2} m\omega^2 q^2\right)}$

$$= \frac{1}{h} \int_{-\infty}^{\infty} e^{-\frac{\beta p^2}{2m}} dp \int_{-\infty}^{\infty} dq \; e^{-\frac{\beta m \omega^2 q^2}{2}}$$

$$= \frac{1}{h} \sqrt{\frac{2\pi m}{\beta}} \sqrt{\frac{2\pi}{\beta m}} \frac{1}{\omega} = \frac{2\pi}{h \beta \omega} = 2\pi \frac{k_B T}{h\omega} = \frac{k_B T}{\hbar \omega}$$

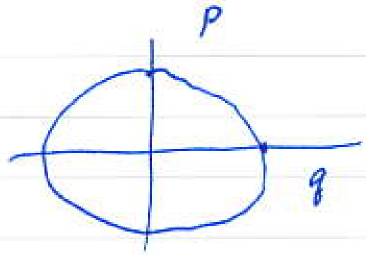
$$F = -k_B T \ln\left(\frac{k_B T}{\hbar \omega}\right)$$

$$S = -\frac{\partial F}{\partial T} = +k_B \ln\left(\frac{k_B T}{\hbar\omega}\right) + k_B$$

$$U = F + TS = k_B T$$

(b)

① $\Gamma = \int_{H<U} dp\, dq$



$$= \text{area of ellipse}$$

$$= \pi \sqrt{\frac{2U}{m\omega^2}} \sqrt{2mU} = \frac{2\pi U}{\omega}$$

$$S = k_B \ln\left(\frac{2\pi U}{\omega}\right)$$

$$\frac{1}{T} = \frac{\partial S}{\partial U} = k_B \frac{1}{U} \qquad \text{ie. } U = k_B T$$

$$F = U - TS = k_B T - T k_B \ln\left(\frac{2\pi k_B T}{\omega}\right)$$

② $\Omega = \Gamma(U+\Delta) - \Gamma(U) = \frac{2\pi\Delta}{\omega}$

$$S = k_B \ln\left(\frac{2\pi\Delta}{\omega}\right)$$

$\frac{1}{T} = \frac{\partial S}{\partial U} = 0 \qquad T \to \infty \qquad U$ ill-defined

F ill-defined

(c) because we did not take $N \to \infty$. $N = 1$

(d) $\Phi = \Gamma(U, N) = \left(\frac{2\pi U}{\omega}\right)^N \cdot \text{const}$

$\Omega \approx \Delta \frac{d\Gamma}{dU} = \text{const}' \left(\frac{2\pi U}{\omega}\right)^{N-1}$

In $N \to \infty$ they are the same.

const $\frac{\pi^{\frac{n}{2}}}{(\frac{n}{2})!}$

4. (a) $T_\ell = T_g$

$P_\ell = T_g$

$\mu_\ell = T_g$

(b) $S = S_\ell + S_g$ $\qquad U_\ell + U_g = U$

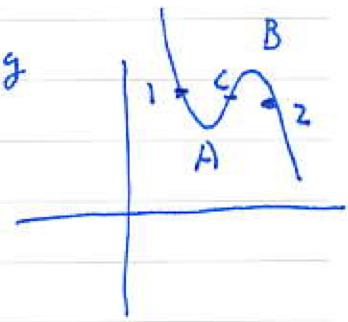
$0 = dS = \frac{\partial S_\ell}{\partial U_\ell} dU_\ell + \frac{\partial S_\ell}{\partial V_\ell} dV_\ell + \frac{\partial S_\ell}{\partial N_\ell} dN_\ell + \frac{\partial S_g}{\partial U_g} dU_g + \ldots$

$= \left(\frac{1}{T_\ell} - \frac{1}{T_g}\right) dU_\ell + \left(\frac{P_\ell}{T_\ell} - \frac{P_g}{T_\ell}\right) dV_\ell + (\mu_\ell - \mu_g) dN_\ell$

$= 0$

$\parallel$

$T_\ell = T_g, \quad P_\ell = P_g, \quad \mu_\ell = \mu_g$



(c) $\mu_g = \mu_g$ means

$\mu_\ell - \mu_g = 0$

using Gibbs-Duhem relation $\quad d\mu = -\frac{S}{N} dT + \frac{V}{N} dP$

on the isotherm curve $dT = 0$

$0 = \mu_\ell - \mu_g = \int_{\mu_\ell}^{\mu_g} d\mu = \int \frac{V}{N} dP = 0 \qquad \int_{1, A, C, B, 2} V dP = 0 \to$ Area I $=$ Area II

2D Ising basic idea.

write the transfer matrix $V = e^{\text{quadratic terms of spin/fermion operator}}$

$$H = -J\sum_{i=1}^{N}\sigma_i\sigma_{i+1} - h\sum_{i=1}^{N}\sigma_i \qquad \beta J = K$$

$$Z = \sum_{\{\sigma\}} \underbrace{e^{\beta h\sigma_1}}_{V_1}\underbrace{e^{K\sigma_1\sigma_2}}_{V_2}\underbrace{e^{\beta h\sigma_2}}_{V_1}\underbrace{e^{K\sigma_2\sigma_3}}_{V_2}\cdots e^{\beta h\sigma_N}e^{K\sigma_N\sigma_1}$$

matrix elements

$$= \sum \langle\sigma_0|V_1|\sigma_1\rangle\langle\sigma_1|V_2|\sigma_2\rangle\langle\sigma_2|V_1|\cdots\quad\cdots|\sigma_0\rangle$$

$$\hat\sigma_z = \begin{pmatrix}1&0\\0&-1\end{pmatrix} \quad \hat\sigma^+ = \begin{pmatrix}0&1\\0&0\end{pmatrix} \quad \hat\sigma^- = \begin{pmatrix}0&0\\1&0\end{pmatrix}$$

$$\hat\sigma_x = \hat\sigma^+ + \hat\sigma^-, \qquad \hat\sigma_y = -i(\hat\sigma^+ - \hat\sigma^-)$$

$$\langle +1|V_1|+1\rangle = e^{\beta h} \qquad \langle +1|V_1|-1\rangle = 0$$
$$\langle -1|V_1|-1\rangle = e^{-\beta h} \qquad \langle -1|V_1|+\rangle = 0$$

$$\langle +1|V_2|+1\rangle = \langle -1|V_2|-1\rangle = e^{K}$$
$$\langle +1|V_2|-1\rangle = \langle -1|V_2|+1\rangle = e^{-K}$$

matrix

$$V_1 = e^{\beta h\hat\sigma_z} = 1 + e^{\beta h}\hat\sigma_z + e^{\beta h}\hat\sigma_z^2 + \cdots = \begin{pmatrix}e^{\beta h}&0\\0&e^{-\beta h}\end{pmatrix}$$

$$V_2 = e^{K}\mathbb{1} + e^{-K}\sigma_x = A e^{K^*\sigma_x} \qquad \sigma_x^2 = 1$$

$$= A\left\{1 + K^*\sigma_x + \frac{1}{2}(K^*\sigma_x)^2 + \frac{(K^*\sigma_x)^3}{3!} + \cdots\right\}$$

$$= A\left\{1 + \frac{1}{2}K^{*2} + \frac{1}{4!}K^{*4} \cdots \left(K^* + \frac{K^{*3}}{3!} + \cdot\right)\sigma_x\right\}$$

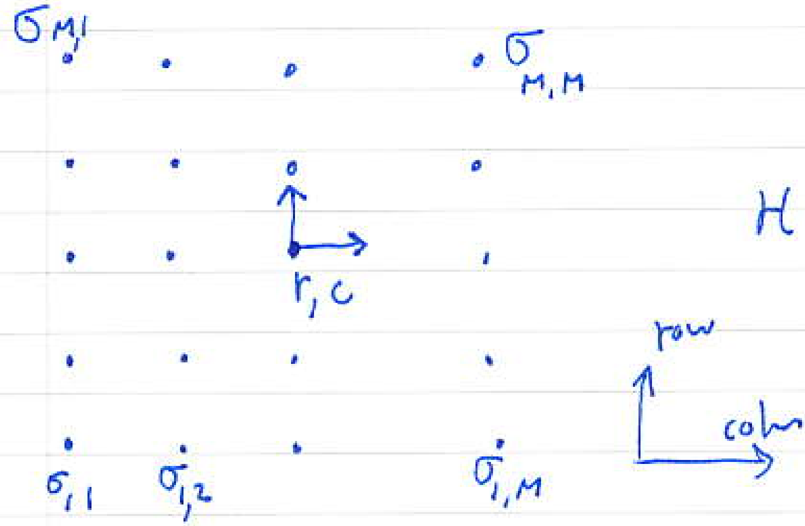
$$= A\cosh K^* + A\sinh K^*\sigma_x$$

$$\rightarrow \quad A\cosh K^* = e^{K}, \quad A\sinh K = e^{-K}$$

$Z = \mathrm{Tr}(V_1 V_2)^N = \mathrm{Tr}(V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}})^N = \lambda_1^N + \lambda_N^N$ ← eigenvalue of V

Date

$$V = V_2^{\frac{1}{2}} V_1 V_2^{\frac{1}{2}} = \sqrt{2\sinh(2K)}\, e^{K^* \hat{\sigma}_x / 2}\, e^{\beta h \hat{\sigma}_z}\, e^{K^* \hat{\sigma}_x / 2}$$



$$H = -J \sum_{rc} \sigma_{r,c}\, \sigma_{r+1,c} - J \sum \sigma_{r,c}\, \sigma_{r,c+1}$$

↙ states of a particular column

2^M basis $|\mu\rangle = |\mu_1 \mu_2 \cdots \mu_M\rangle = |\mu_1\rangle |\mu_2\rangle \cdots |\mu_M\rangle$

$\hat{\sigma}_{jx}$ $\hat{\sigma}_{jy}$ $\hat{\sigma}_{jz}$ $j = 1, 2, \cdots M$ acts on $|\mu\rangle$

$[\hat{\sigma}_{j\alpha}, \hat{\sigma}_{m\beta}] = 0$ if $j \neq m$

2D Ising → quasi 1D spin chain

$$Z = \sum_{\{\sigma\}} e^{\beta J \sum_{rc} \sigma_{rc} \sigma_{r+1 c} + \beta J \sum_{rc} \sigma_{r,c} \sigma_{r,c+1}}$$

↑ ~~colm~~ c colm ↑ r row

$$= \sum_{\{\sigma\}} \underbrace{e^{\beta J \sum_r \sigma_{r,1} \sigma_{r+1,1}}}_{\text{column 1}}\ \underbrace{e^{\beta J \sum \sigma_{r,1} \sigma_{r,2}}}_{\text{betw colm 1 \& 2}}\ \underbrace{e^{\beta J \sum_r \sigma_{r,2} \sigma_{r+1,2}}}_{\text{column 2}}\ \underbrace{\cdots}_{\text{colm 3}}$$

V_1 V_2

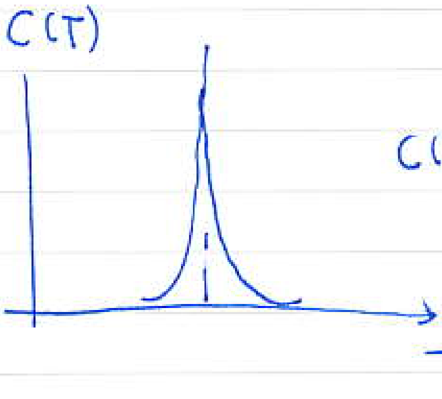
$$V_1 = e^{K \sum_j \hat{\sigma}_{jz} \hat{\sigma}_{j+1,z}} \qquad V_2 = (2\sinh 2K)^{\frac{M}{2}} e^{\left(K^* \sum_{j=1}^{M} \hat{\sigma}_{jx}\right)}$$

onsager exact solution 1944

free energy

$$\frac{\beta F(h=0, T)}{N} = -\ln(2\cosh 2K) - \frac{1}{\pi}\int_0^{\frac{\pi}{2}} d\theta \ \ln \frac{1+\sqrt{1-q^2\sin^2\theta}}{2}$$

$$q = \frac{2\sinh 2K}{\cosh^2 2K}$$



$$C(T) = -\frac{2}{\pi}k_B\left(\frac{2J}{k_B T_c}\right)^2 \ln\left|1-\frac{T}{T_c}\right| + \text{const}$$

$$\frac{k_B T_c}{J} = 2.269185$$

or $\sinh(2K_c) = 1$

due to C N Yang: 1952

$$\frac{M}{N} = \left(1-\frac{1}{\sinh^4(2K)}\right)^{\frac{1}{8}} \quad T < T_c$$

$$\beta = \frac{1}{8}$$

$$\chi = \left.\frac{\partial m}{\partial h}\right|_{h=0} \approx |T-T_c|^{-\frac{7}{4}} \qquad \gamma = \frac{7}{4}$$

onsager conjectured it 1949

Date

$$Q(T,V,N) = \lambda^{3N} Q(T\lambda^{-\gamma}, V\lambda^{-3}, N)$$

$$Q(T,V,N) = T^{\frac{3N}{\gamma}} Q(1, VT^{-\frac{3}{\gamma}}, N)$$

$$P = -\frac{\partial F}{\partial V} = -\frac{\partial}{\partial V}(-k_B T \ln Q)$$

$$f(\lambda VT^{-\frac{3}{\gamma}}, \lambda N) = \lambda^{0} f(VT^{-\frac{3}{\gamma}}, N)$$

$$= k_B T \frac{\partial}{\partial V}\left[\ln Q(1, VT^{-\frac{3}{\gamma}}, N) + \right]$$

$$= k_B T\left[\left(\ln Q(1, VT^{-\frac{3}{\gamma}}, N)\right)' T^{-\frac{3}{\gamma}}\right.$$

because it is intensive we must have

$$= T^{1-\frac{3}{\gamma}} f(VT^{-\frac{3}{\gamma}}, N) \to T^{1-\frac{3}{\gamma}} g\left(\frac{V}{N} T^{-\frac{3}{\gamma}}\right)$$

(P

12 March 07

Assignt 3.

Date

① 2.3 $$Z(T,V,N) = \frac{1}{h^{3N} N!} \int e^{-\beta \mathcal{H}} d^3\vec{r}_1 d^3\vec{r}_2 \cdots dr_N d^3\vec{p}_1 \cdots d^3\vec{p}_N$$

$$= \frac{1}{N!\, h^{3N}} \left[\int_{-\infty}^{\infty} e^{-\beta \frac{p^2}{2m}} dp \right]^{3N} \int e^{-\beta U} d^3\vec{r}_1 \cdots d^3\vec{r}_N$$

$$= \frac{1}{N!\, h^{3N}} \left(2\pi m k_B T \right)^{\frac{3N}{2}} \cdot Q_N \qquad \lambda^{-1} = \frac{\sqrt{2\pi m k_B T}}{h}$$

$$= \frac{1}{N!} (\lambda)^{-3N} Q_N$$

$P = -\frac{\partial F}{\partial V}$ T-depen do not contribute

$$Q(T,V,N) = \int_V d\vec{r}_1 \cdots \int d\vec{r}_N \, e^{-\beta U(\vec{r}_1, \vec{r}_2 \cdots \vec{r}_N)}$$

$\int_0^L dx' \rightarrow \lambda \int_0^{L} d\lambda x$

$r_n' = \lambda r_n$

$$Q(T,V,N) = \lambda^{3N} \int_{V\lambda^{-3}} d\vec{r}_1 \cdots \int d\vec{r}_N \, e^{-\beta \lambda^{\gamma} U(\vec{r}_1 \cdots \vec{r}_N)}$$

$$= \lambda^{3N} Q(T\lambda^{-\gamma}, V\lambda^{-3}, N)$$

$\frac{V}{N} = v \qquad Q(T, v) = \lambda^{3N} Q(T\lambda^{-\gamma}, v\lambda^{-3}) \qquad \lambda = v^{\frac{1}{3}}$

true for any λ, change $v\lambda^{-3} = 1$, ~~we get~~ or $T\lambda^{-\gamma} = 1$

$$Q(T,v) = v^N g(T v^{-\frac{\gamma}{3}}) = T^{\frac{-3N}{\gamma}} h(v T^{-\frac{3}{\gamma}}) \qquad \lambda = T^{\frac{1}{\gamma}}$$

$$P = -\frac{\partial}{\partial V} \underline{(-k_B T)\left[\ln Q + \text{const}\right]} = k_B T \frac{1}{Q} \frac{\partial Q}{\partial V} = k_B T \frac{1}{Q} \frac{\partial Q}{\partial v} \cdot \frac{1}{N}$$

$$P = k_B T \, \frac{1}{N} \left[\frac{\partial \ln Q}{\partial v} \right]$$

$$\cancel{k_B T N \frac{\partial}{\partial v}[N \ln v +}$$

Date

$$= k_B T \frac{1}{N} \left[\frac{\partial}{\partial v} \ln \left(T^{-\frac{3N}{\gamma}} h(v T^{-\frac{3}{\gamma}}) \right) \right]$$

$$= k_B T \frac{1}{N} h'(v T^{-\frac{3}{\gamma}}) \, T^{-\frac{3}{\gamma}} = T^{1-\frac{3}{\gamma}} f\left(\frac{V}{N} T^{-\frac{3}{\gamma}}\right)$$

2.7. (a) $\omega_k = ck$

$$Z = \sum_{n_k = 0,1,2\ldots} e^{-\beta \sum_k \hbar \omega_k n_k} \quad \cancel{= \int \frac{2V}{(2\pi)^3} d^3\vec{k}}$$

$$= \prod_k \frac{1}{1 - e^{-\beta \hbar \omega_k}}$$

$$F = -k_B T \ln Z = -k_B T \ln \prod_k \frac{1}{1 - e^{-\beta \hbar \omega_k}}$$

$$= -k_B T \sum_k \left(-\ln(1 - e^{-\beta \hbar \omega_k}) \right)$$

$$= k_B T \int \frac{(2V)}{(2\pi)^3} d^3\vec{k} \, \ln(1 - e^{-\beta \hbar \omega_k})$$

$$k = \frac{\omega}{c}$$

$$= k_B T \int \frac{(2V)}{(2\pi)^3} 4\pi k^2 dk \, \ln(1 - e^{-\beta \hbar \omega_k})$$

$$= \frac{V k_B T \cdot \cancel{2} \cdot 4}{\cancel{8} \pi^2 c^3} \int \omega^2 d\omega \, \ln(1 - e^{-\beta \hbar \omega})$$

$$= \frac{V k_B T}{\pi^2 c^3} \int_0^\infty d\omega \cdot \omega^2 \ln(1 - e^{-\beta \hbar \omega})$$

$$= \frac{V k_B T}{\pi^2 c^3} \left(-\frac{\pi^4}{45 (\beta \hbar)^3} \right) = -\frac{\pi^2 V}{45 c^3 \hbar^3 \beta^4}$$

(b)

$$P = -\frac{\partial F}{\partial V} = \frac{-k_B T}{\pi^2 c^3} \int_0^\infty d\omega \cdot \omega^2 \ln\left(1 - e^{-\beta\hbar\omega}\right) = \frac{\pi^2}{45 c^3 \hbar^3 \beta^4}$$

Date

$$U = \frac{\partial \beta F}{\partial \beta} = \frac{\partial}{\partial \beta}\left(\frac{V}{\pi^2 c^2} \int_0^\infty d\omega \cdot \omega^2 \ln\left(1 - e^{-\beta\hbar\omega}\right)\right)$$

$$= \frac{V}{\pi^2 c^3} \int_0^\infty d\omega \cdot \omega^2 \frac{e^{-\beta\hbar\omega} \cdot \hbar\omega}{1 - e^{-\beta\hbar\omega}}$$

$$= \frac{V}{\pi^2 c^3} \int_0^\infty d\omega \cdot \omega^2 \cdot \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} = \frac{3}{45} \frac{\pi^2 V}{c^3 \hbar^3 \beta^4}$$

$$PV = -\frac{k_B T V}{\pi^2 c^3} \int_0^\infty d\omega \cdot \omega^2 \ln\left(1 - e^{-\beta\hbar\omega}\right)$$

$$= \frac{k_B T V}{\pi^2 c^3} \int_0^\infty \cancel{\omega^2 d} \ln\left(1 - e^{-\beta\hbar\omega}\right) d\frac{\omega^3}{3}$$

$$= \frac{k_B T V}{\pi^2 c^3} \left[+ \frac{\omega^3}{3} \ln\left(1 - e^{-\beta\hbar\omega}\right)\Big|_0^\infty + \int_0^\infty \frac{\omega^3}{3} \frac{(-e^{-\beta\hbar\omega}(-\beta\hbar))}{1 - e^{-\beta\hbar\omega}} d\omega \right]$$

$$= \frac{1}{3} \frac{V}{\pi^2 c^3} \int_0^\infty \frac{\hbar\omega}{e^{\beta\hbar\omega} - 1} \omega^2 d\omega = \frac{1}{3} U$$

$\frac{1}{3}$ vs. $\frac{2}{3}$. disperse relation is different!

13 March 07

Date

Scaling of free energy

$$f(t,h) = \frac{F(T,h)}{N}$$ free energy per spin

$$t = \frac{T-T_c}{T_c}$$ $t=0$ mean critical pt

$$f(t,h) = \underset{b}{L^{-d}} f(L^{y}t, L^{x}h)$$ for any L — L for system size

+ regular (analytic piece)

Take $L^{y}t = 1$ — d : dimension of system

$$L = t^{-\frac{1}{y}}$$ use "b" for L here

$$f(t,h) = t^{+\frac{d}{y}} f(1, t^{-\frac{x}{y}}h)$$ b : linear scaling factor

$$= t^{+\frac{d}{y}} \hat{f}(t^{-\frac{x}{y}}h)$$

$$m = -\frac{\partial f}{\partial h} = t^{\frac{+d}{y}} \hat{f}'(t^{-\frac{x}{y}}h) \cdot t^{-\frac{x}{y}} \Big|_{h=0} = t^{-\frac{-d+x}{y}} \hat{f}'(0) \propto t^{\beta}$$

$$\beta = -\cancel{\frac{-d+x}{y}} = \frac{-x+d}{y}$$

$$\chi = \frac{\partial m}{\partial h} = t^{-\frac{-d\pm x}{y}} \hat{f}''(t^{-\frac{x}{y}}h)\, t^{-\frac{x}{y}} \Big|_{h=0} = t^{-\frac{(-d)+2x}{y}} \propto t^{-\gamma}$$

$$\gamma = \frac{-d+2x}{y}$$

$$m = t^{\frac{d-x}{y}} \hat{f}'(t^{-\frac{x}{y}}h) = h^{\frac{d-x}{x}} \left(t^{-\frac{x}{y}}h\right)^{-\frac{y}{x}\left(\frac{d-x}{y}\right)} \hat{f}(t^{-\frac{x}{y}}h) \Big|_{t=0}$$

$$\propto h^{1/\delta}$$

$$\delta = \frac{x}{d-x}$$

$$\frac{\partial f}{\partial t} = -S$$

heat capacity ~~$dU = -SdT$~~

$$dF = -S\,dT - M\,dh$$

$$U = F + TS$$

$$dU = \underbrace{T\,dS}_{dQ} - M\,dh$$

heat capacity near T_c

$$C_h = \frac{dQ}{dT}\Big|_{h=0} = T\frac{dS}{dT} \simeq T_c \frac{\partial S}{\partial T}\Big|_{h=0}$$

$$c_h = \frac{C_h}{N} = T_c\left(-\frac{\partial^2 f}{\partial t^2}\right)\Big|_{h=0} \propto \frac{\partial}{\partial t}\left[\frac{d}{y} t^{\frac{d}{y}-1} \hat{f}(t^{-\frac{x}{y}}h) + t^{\frac{d}{y}} \hat{f}'(t^{-\frac{x}{y}}h)\left(-\frac{x}{y}t^{-\frac{x}{y}-1}\right)\right.$$

$$\propto t^{\frac{d}{y}-2}\hat{f}(0) \leftarrow h=0 \quad \propto t^{-\alpha}$$

$$\alpha = 2 - \frac{d}{y}$$ hyperscaling

$$\alpha + 2\beta + \gamma = 2 - \frac{d}{y} + 2\left(\frac{-x+d}{y}\right) + \frac{-d+2x}{y}$$

$$= 2 + \frac{-d - 2x + 2d - d + 2x}{y} = 2$$

$$\boxed{\alpha + 2\beta + \gamma = 2}$$ Rushbrooke's scaling law

$$\beta(\delta - 1) = \frac{d-x}{y}\left(\frac{x}{d-x} - 1\right) = \frac{\cancel{d-x}}{y}\,\frac{x-d+x}{\cancel{d-x}} = \frac{2x-d}{y} = \gamma$$

$$\boxed{\beta(\delta-1) = \gamma}$$ Widom's scaling law

concept of Universality

critical exponents only depends on

1. dimensionality d
2. spin-dimension n
3. range of interaction

critical exponents

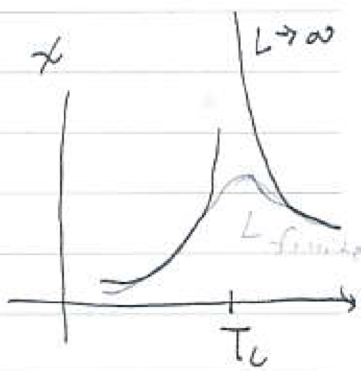
Date

exponent	definitions	2D Ising	3D Ising /fluid	mean-field
α	$C \sim \lvert t\rvert^{-\alpha}$	0	0.12	?
β	$m \sim \lvert t\rvert^{\beta}$	$\frac{1}{8}$	0.32	$\frac{1}{2}$
γ	$\chi \sim \lvert t\rvert^{-\gamma}$	$\frac{7}{4}$	1.25	1
δ	$h \sim m^{\delta}$	15	5.0	3
$\nu = \frac{1}{y}$	$\xi \sim \lvert t\rvert^{-\nu}$	1	0.63	$\frac{1}{2}$
η	$G(r) \sim \frac{e^{-\frac{r}{\xi}}}{r^{d-2+\eta}}$	$\frac{1}{4}$	0.06	0

$$\chi = \int d^d r\, G(r) = \int \frac{e^{-\frac{r}{\xi}}}{r^{d-2+\eta}} r^{d-1} dr \approx \xi^{2-\eta} \simeq |t|^{-\nu(2-\eta)} \sim |t|^{-\gamma}$$

$$\boxed{\gamma = \nu(2-\eta)}$$ Fisher scaling law

hyperscaling (Josephson) $\boxed{d\nu = 2 - \alpha}$

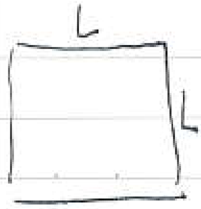


Finite-size Scaling

$$f(t, h, L) = b^{-d} f(b^{y} t,\ b^{x} h,\ b/L)$$

size

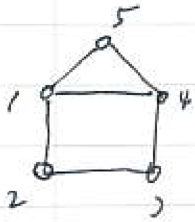
finite-size rounding, e.g.

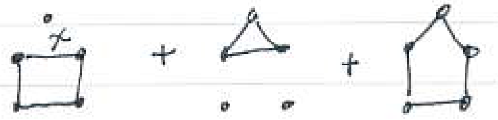


$$\chi(t, h=0, L) = L^{\gamma/\nu}\, \tilde{\chi}(t L^{1/\nu})$$

~~Renormalization group~~ method. $N=5$ $L=6$ $x = \tanh K$

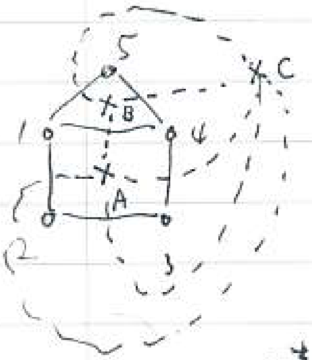
Date



$Z = 2^5 (\cosh K)^6 \Big(1 +$  $\Big)$

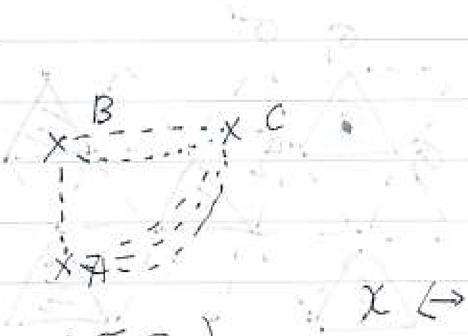
$= 2^5 (\cosh K)^6 (1 + x^4 + x^3 + x^5)$

$$Z = \sum_{\{\sigma_1 \sigma_2 \cdots \sigma_5\}} e^{K(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_4 + \sigma_1\sigma_4 + \sigma_1\sigma_5 + \sigma_5\sigma_4)}$$



$N^* = 3$
$L^* = L = 6$

dual Lattice

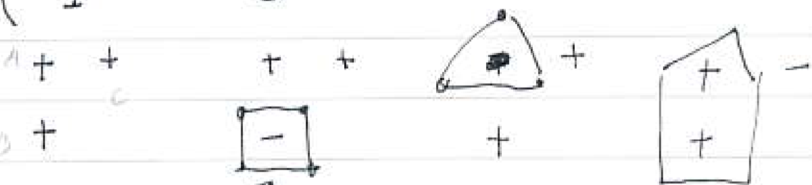


$x \leftrightarrow e^{-2K}$

$$Z^* = \sum_{\sigma_A \sigma_B \sigma_C} e^{K(\sigma_A\sigma_B + 2\sigma_B\sigma_C + 3\sigma_A\sigma_C)}$$

$\downarrow$

$= 2 e^{K\cdot 6} \Big(1 + e^{-8K} + e^{-6K} + e^{-10K} \Big)$



$2^3 = 8$ ✓

wall

boundary connects + with −

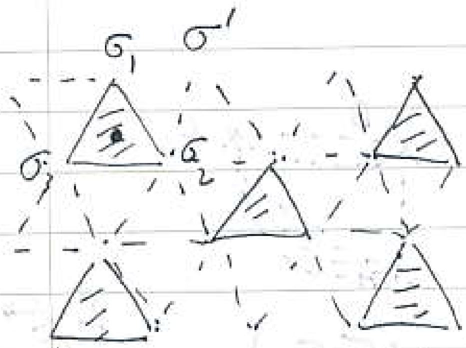
We see p $V(r) = p^*(r)$

$r = 0, 4, 3, 5$

The low-temperature expansion coefficient on dual lattice p^* is the same as the high-temperature ~~resel~~ result of the original lattice

Date

Block spin transform on triangular lattice

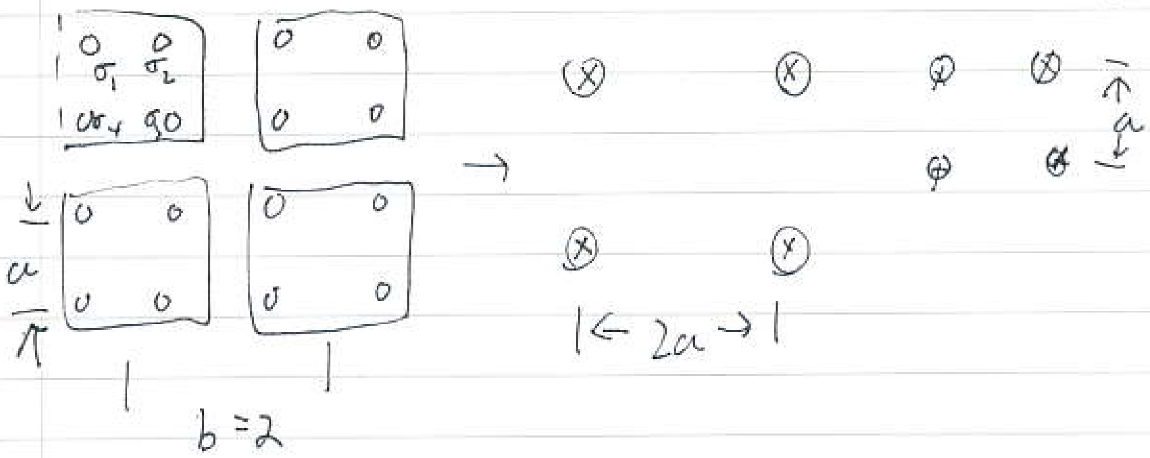


$$P(\sigma', \sigma) = \prod \frac{1}{2}\left[1 + \sigma'(\sigma_1 + \sigma_2 + \sigma_3 - \sigma_1\sigma_2\sigma_3)\frac{1}{2}\right]$$

RG method

Kadanoff block spin transformation

Scaling picture
scaling invariant at T_c



new spin $\sigma_1' =$ majority of $(\sigma_1\, \sigma_2\, \sigma_3\, \sigma_4)$
or sign of $\sum_{i=1}^{4} \sigma_i$.

$$H = \sum_\alpha K_\alpha S_\alpha \qquad S_\alpha = \prod_{i \in I_\alpha} \sigma_i \qquad I_\alpha$$

empty set
n.n.
site site

$$= K_0 + K_1 \sum_i \sigma_i + K_2 \sum_{\langle ij \rangle} \sigma_i \sigma_j + K_3 \sum \sigma_i \sigma_j \sigma_k + \cdots$$

$$Z_N = \sum_{\{\sigma\}} e^{-H(\sigma)} \qquad Z'_{N'} = \sum_{\{\sigma'\}} e^{-H'(\sigma')}$$ renormalize H'

$$Z_N = Z'_{N'}$$

$$e^{-H'(\sigma')} = \sum_{\{\sigma\}} P(\sigma', \sigma)\, e^{-H(\sigma)}$$

① Block spin
② decimation

$$\sum_{\sigma'} P(\sigma', \sigma) = 1 \qquad P(\sigma', \sigma) \geq 0$$

RG transfm $H(\sigma) \to H'(\sigma')$ or $\{K_i\} \to \{K_i'\}$

$\vec{K}' = f(\vec{K})$ $\vec{K}'' = f(\vec{K}')$ $\cdots$ $\vec{K}_{n+1}^{(n+1)} = f(\vec{K}_n^{(n)})$

$n \to \infty$ fixed point. $\vec{K}^* = f(\vec{K}^*)$

Date

Expanding around fixed pt.

$$\delta \vec{K}_{n+1}^{(n+1)} = \vec{K}_{n+1}^{(n+1)} - \vec{K}^* = f(\vec{K}_n) - f(\vec{K}^*)$$
$$= W(\vec{K}_n^{(n)} - \vec{K}^*)$$

$\rightarrow$ $\delta \vec{K}_{n+1}^{(n+1)} = \vec{W} \delta \vec{K}_n^{(n)}$ $\leftarrow$ linearized transform

Let $\phi W = \lambda \phi$ left eigen vector of W

$$v^{(n)} = \sum_\alpha \phi_\alpha (\delta K^{(n)})_\alpha$$
$$v^{(n+1)} = \sum_\alpha \phi_\alpha (\delta K^{(n+1)})_\alpha = \sum \underbrace{\phi_\alpha W_{\alpha\beta}} \delta K_\beta^{(n)} = \lambda \sum \phi_\beta \delta K_\beta^{(n)}$$
$$= \lambda v^{(n)}$$

$\rightarrow$ new scaling field

original new variable

$\lambda > 1$ relevant $\{K\} \rightarrow \{v\}$

$\lambda < 0$ irrelevant

$\lambda = 0$ marginal

$\lambda = b^y \leftarrow$ critical exponent

free magnetic

In symbol cases $v_1 = t = \frac{T - T_c}{T}$, $v_2 = h$

RG transform $t' = \lambda_T t = b^{y_T} t$ $y_T = y$

$h' = \lambda_H h = b^{y_H} h$ $y_H = x$

$Z_N(K) = Z'_{N'}(K')$ $\frac{N'}{N} = b^{-d}$

$N f(\{v\}) = N' f(\{v'\}) \Rightarrow f(t, h) = b^{-d} f(b^{y_T} t, b^{y_H} h)$

At fixed point $\xi = 0$, or ∞

$$\xi(t,h) = b\,\xi(b^y t, b^x h)$$

Date

n iteration $\quad \xi(0,0) = b^n \xi(0,0)$

Field-theoretic approach

Ginsburg-Landau-Wilson model $\qquad \phi^4$-theory

$$H(\phi) = \int d^d x \left\{ \frac{1}{2}(\nabla\phi)^2 + \frac{1}{2} r_0 \phi^2 + \frac{u_0}{4} \phi^4 \right\} \qquad \phi(x)$$

Universality for the RG point of view.

RG results $\quad$ (ε-expansion) $\qquad \varepsilon = 4-d$

$$\beta = \frac{1}{2} - \frac{3\varepsilon}{2(n+8)} + \frac{\varepsilon^2 (n+2)(2n+1)}{2(n+8)^3} + \cdots$$

upto ε^5 are presently known

$$\nu = \frac{1}{2} + \frac{\varepsilon(n+2)}{4(n+8)} + \frac{\varepsilon^2 (n+2)}{8(n+8)^3}(n^2+23n+60) + \cdots$$

K Wilson find to ε^2 order

n dimension of the spin $\quad n=1$ Ising

$n=2$ XY model

$n=3$ Heisenberg model

Tutorial 4

4. $i = 1, 2, \ldots N$, $j = 1, 2$, $\sigma_{i,j}$

$$Z = \sum_{\{\sigma\}} e^{K \sum_{i=1}^{N} (\sigma_{i,1}\sigma_{i+1,1} + \sigma_{i,2}\sigma_{i+1,2} + \sigma_{i,1}\sigma_{i,2})}$$

$$= \sum_{\{\sigma\}} \prod_i e^{K(\sigma_{i,1}\sigma_{i+1,1} + \sigma_{i,2}\sigma_{i+1,2} + \frac{1}{2}\sigma_{i,1}\sigma_{i,2} + \frac{1}{2}\sigma_{i+1,1}\sigma_{i+1,2})}$$

$$V(\sigma_1 \sigma_2 ; \sigma_1' \sigma_2') = e^{K(\sigma_1\sigma_1' + \sigma_2\sigma_2' + \frac{1}{2}\sigma_1\sigma_2 + \frac{1}{2}\sigma_1'\sigma_2')}$$

$$V = \begin{array}{c} \\ ++ \\ +- \\ -+ \\ -- \\ \uparrow\uparrow \\ \sigma_1\sigma_2 \end{array} \begin{array}{c} \sigma_1'\sigma_2' \\ \begin{array}{cccc} ++ & +- & -+ & -- \end{array} \\ \begin{bmatrix} e^{3K} & 1 & 1 & e^{-K} \\ 1 & e^{K} & e^{-3K} & 1 \\ 1 & e^{-3K} & e^{K} & 1 \\ e^{-K} & 1 & 1 & e^{3K} \end{bmatrix} \\ \\ \\ \end{array}$$

$2 \quad -1$

$1 + 1 + \frac{1}{2}(-1-1)$

$2 + -1$

largest eigen value

$$\lambda_{Max} = \frac{1}{2} e^{-4K} \left(e^{K} + e^{3K} + e^{5K} + e^{7K} + e^{K}(1 + e^{2K})\sqrt{1 - 4e^{K} + 10e^{4K} - 4e^{6K} + e^{8K}} \right)$$

$$Z = \mathrm{Tr}(V^N) = \lambda_1^N + \lambda_2^N + \lambda_3^N + \lambda_4^N$$

$N \to \infty$ $\quad F = -N k_B T \ln \lambda_{Max}$

eigenvalues $\det(V - \lambda I) = 0$ $\qquad e^K = x$

Date

$$\det \begin{bmatrix} e^{3K}-\lambda & 1 & 1 & e^{-K} \\ 1 & e^{K}-\lambda & e^{-3K} & 1 \\ 1 & e^{-3K} & e^{K}-\lambda & 1 \\ e^{-K} & 1 & 1 & e^{3K}-\lambda \end{bmatrix} = 0$$

$$\begin{vmatrix} x^3-\lambda & 1 & 1 & x^{-1} \\ 1 & x-\lambda & x^{-3} & 1 \\ 1 & x^{-3} & x-\lambda & 1 \\ x^{-1} & 1 & 1 & x^3-\lambda \end{vmatrix} = 0$$

$|A_{ij}|$ minor

$A_{ij} = (-1)^{i+j} |A_{ij}|$ ← cofactor

Laplace expansion ~~1st row~~ $\qquad |A| = \sum_j a_{ij} A_{ij}$ fixing i

$$= (x^3-\lambda) \begin{vmatrix} x-\lambda & x^{-3} & 1 \\ x^{-3} & x-\lambda & 1 \\ 1 & 1 & x^3-\lambda \end{vmatrix} - \begin{vmatrix} 1 & x^{-3} & 1 \\ 1 & x-\lambda & 1 \\ x^{-1} & 1 & x^3-\lambda \end{vmatrix} + \begin{vmatrix} 1 & x-\lambda & 1 \\ 1 & x^{-3} & 1 \\ x^{-1} & 1 & x^3-\lambda \end{vmatrix}$$

$$- x^{-1} \begin{vmatrix} 1 & x-\lambda & x^{-3} \\ 1 & x^{-3} & x-\lambda \\ x^{-1} & 1 & 1 \end{vmatrix}$$

$$= (x^3-\lambda)\left[(x-\lambda)^2(x^3-\lambda) + 2x^{-3} - (x-\lambda) - x^{-6}(x^3-\lambda) - (x-\lambda) \right]$$

$$- \left[(x-\lambda)(x^3-\lambda) + x^{-3}(x^3-\lambda) + x^{-1}(x-\lambda) - \cdots \right]$$

$\cdots$

$$= e^{-8K}(-1 + e^{4K} - e^{K}\lambda)(-1 + e^{4K} - e^{3K}\lambda) \times ($$
$$1 - 2e^{4K} + e^{8K} - (e^{K} + e^{3K} + e^{5K} + e^{7K})\lambda + e^{4K}\lambda^2)$$

Date

$$\lambda_1 = e^{3K} - e^{-K}$$

$$\lambda_2 = e^{K} - e^{-3K}$$

$$\lambda_{3,4} = \frac{1}{2e^{4K}}\left[e^{K} + e^{3K} + e^{5K} + e^{7K} \pm \sqrt{(e^{K}+e^{3K}+e^{5K}+e^{7K})^2 - 4\times(1-2e^{4K}+e^{8K})e^{4K}} \right]$$

as $K \to \infty$ $\quad \lambda_1 \propto e^{3K}$

$\lambda_2 \propto e^{K}$

$\lambda_{3,4} \propto e^{3K}$

5. (a) $$\langle M \rangle = \left\langle \sum_{i=1}^{N} \sigma_i \right\rangle = \frac{1}{Z} \sum_{\{\sigma\}} \underbrace{\left(\sum_{i=1}^{N} \sigma_i\right)}_{M} e^{K\sum_{\langle ij \rangle}\sigma_i\sigma_j + \beta h \underbrace{\sum_i \sigma_i}_{M}}$$

$$\chi = \frac{\partial \langle M \rangle}{\partial h}\Big|_{h=0} = \frac{\partial}{\partial h}\left(\frac{1}{Z}\sum_{\{\sigma\}} M(\sigma)\, e^{K\sum_{\langle ij \rangle}\sigma_i\sigma_j + \beta h M(\sigma)} \right)$$

$$= \frac{1}{Z}\sum_{\{\sigma\}} M(\sigma) \frac{\partial}{\partial h} e^{K\sum\sigma_i\sigma_j + \beta h M(\sigma)} - \frac{\sum M(\sigma) e^{K\Sigma + \beta h M}}{Z^2} \frac{\partial}{\partial h} Z$$

$$= \frac{1}{Z}\sum_{\{\sigma\}} M(\sigma)\cdot \beta M(\sigma)\, e^{K\sum\sigma_i\sigma_j + \beta h M(\sigma)} - \frac{\sum M(\sigma) e^{K\sum\sigma_i\sigma_j + \beta h M(\sigma)}}{Z} \frac{1}{Z}\frac{\partial Z}{\partial h}$$

$$= \beta \langle M(\sigma)^2 \rangle - \langle M \rangle \frac{1}{Z}\frac{\partial Z}{\partial h}$$

$$\frac{1}{Z}\frac{\partial Z}{\partial h} = \frac{1}{Z}\sum \frac{\partial}{\partial h} e^{K\sum_{\langle ij \rangle}\sigma_i\sigma_j + \beta h \sum_i \sigma_i} = \frac{1}{Z}\sum \beta M(\sigma)\, e^{K\sum\sigma_i\sigma_j + \beta h M(\sigma)}$$

$$= \beta \langle M \rangle$$

So $$\chi = \beta\left[\langle M(\sigma)^2 \rangle - \langle M(\sigma) \rangle^2\right] \qquad \beta = \frac{1}{k_B T}$$

(b) $\langle M \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \sum_{i=1}^{N} \sigma_i \, e^{K \sum_{\langle ij \rangle} \sigma_i \sigma_j}$ set $h = 0$

Date

$$= \frac{1}{Z} \sum_{\{\sigma\}} \left(\sum_{i=1}^{N} \sigma_i \right) (\cosh^L K) \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j \tanh K) = 0$$

because there are always odd # of spins at each site

$$\langle M^2 \rangle = \frac{1}{Z} \sum_{\{\sigma\}} \left(\sum_{i=1}^{N} \sigma_i \right)^2 (\cosh^L K) \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j \tanh K)$$

$$Z = \sum_{\{\sigma\}} (\cosh^L K) \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j \tanh K)$$

$$= \frac{\sum_{\{\sigma\}} \sum_{k\ell}^{N} \sigma_k \sigma_\ell \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j x)}{\sum_{\{\sigma\}} \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j x)}$$

$k = \ell$

$$= \sum_{k=1}^{N} \sigma_k^2 \sum_{\{\sigma\}} \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j x) \Big/ \sum_{\{\sigma\}} \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j x)$$

$= N +$

$\sum_{\{\sigma\}} \prod_{\langle ij \rangle} (1 + \sigma_i \sigma_j x) = 1 + \cdots x^4$

k ℓ are nearest neigh

# of bonds

$= N + \underbrace{x \cdot N \cdot d \cdot 2}$ ← d-dimensional hypercubic lattice

$+ x^2 \cdot N \cdot \frac{2d(2d-1)}{2} \cdot 2 + \cdots$

$\sum_{k\ell}$

$\chi = \frac{N}{k_B T} \left(\cancel{1 + 2d \cdot x + \cdots} \right)$ — k can be on 1st or second sites

for each graph of $\prod(\cdots)$ there are two terms contributing

$$\chi = \frac{N}{k_B T} \left(1 + 2d \cdot x + 2d(2d-1) x^2 + \cdots \right)$$

$$= \frac{N}{k_B T} \left(1 + z \cdot x + z(z-1) x^2 + \cdots \right)$$

$z = 2d$ is coordination number

Q7 $E = -\sum \mu_B H \cos\theta$

Date

(a) $Z = z^N \qquad z = \int e^{-\beta E} \sin\theta \, d\theta \, d\varphi$

$$= 2\pi \int_0^\pi e^{\beta \mu_B H \cos\theta} \sin\theta \, d\theta$$

$$= 2\pi \int_0^\pi e^{\beta \mu_B H \cos\theta} [-d\cos\theta] \qquad \cos\theta = x$$

$$= 2\pi \left[-\int_1^{-1} e^{\beta \mu_B H x} dx \right] = \frac{2\pi(-1)}{\beta \mu_B H} \left[e^{\beta \mu_B H x} \right]_1^{-1}$$

$$= \frac{2\pi(-1)}{\beta \mu_B H} \left[e^{-\beta \mu_B H} - e^{\beta \mu_B H} \right] = \frac{4\pi}{\beta \mu_B H} \sinh(\beta \mu_B H)$$

$x \to 0 \qquad \sinh x = x + \frac{1}{6} x^3 + \cdots$

(b) $F = -k_B T \ln z^N$

$$= -N k_B T \ln \frac{2\pi}{\beta \mu_B H} \sinh(\beta \mu_B H)$$

$$= -N k_B T \left[\ln\left((2\pi)\left(1 + \frac{1}{6} \cancel{x} (\beta \mu_B H)^2 + \cdots \right] \right.\right.$$

$$= -N k_B T \left(\ln(2\pi) + \frac{1}{6} (\beta \mu_B H)^2 + \cdots \right)$$

$$= -N k_B T \cdot C - \frac{1}{6} N \frac{(\mu_B H)^2}{k_B T} + \cdots$$

$$S = -\frac{\partial F}{\partial T} = N k_B C + \left(-\frac{1}{6}\right) N \frac{(\mu_B H)^2}{k_B T^2}$$

$$= N k_B \left(C - \frac{1}{6} \left(\frac{\mu_B H}{k_B T} \right)^2 \right)$$

(c) $\Delta Q(B \to C) = 0 \qquad \Delta Q = T \Delta S \qquad dQ = T dS$

$$\Delta Q(A \to B) = T_1 (\Delta S) = T_1 \left(-\frac{N \mu_B^2}{6 k_B T_1^2} (H_2^2 - H_1^2) \right)$$

released

$$\Delta Q = \frac{N}{6} \frac{\mu_B^2}{k_B T_1} (H_2^2 - H_1^2) > 0$$

D (NaCl in water) $\sim 1.2 \times 10^{-10}$ m^2/s $\qquad \langle x^2 \rangle \sim Dt$

gas typical 10^{-6} $\Big\}$ m^2/s

solid in solid 10^{-12}

Date

R. Kubo, M. Toda, N. Hashi[tsume]
"Statistical physics II"

R. Zwanzig, "Nonequilibrium Statistical Mechanics"

N. Pottier, "Nonequilibrium statistical physics"

Einstein 1905

Smoluchowski

21 March 07

Browian motion

① pollen floating in water making irregular motion (1827)

A large number of Brownian

② mirror hits by air molecules mounted on suspension fiber

Fick's law

③ noises in electric circuts

$$j = -D\frac{\partial n}{\partial x}$$ diffusion constant

$n(x)$ 1D (3D is similar)

$$\frac{\partial n}{\partial t} + \nabla\cdot j = 0$$ continuity / conservation of particles

→ diffusion Eq. $\frac{\partial n}{\partial t} = D\frac{\partial^2 n}{\partial x^2}$

solution — transit from $(x_0\, t_0)$ to $x\, t$

$$n(x,t) = \int \underbrace{n(x_0, t_0)}_{\text{initial density}} P(x_0, t_0 | x, t)\, dx_0$$

for open b.c.

$$P(x_0, t_0 | x, t) = \frac{1}{\sqrt{4\pi D(t-t_0)}} e^{-\frac{(x-x_0)^2}{4D(t-t_0)}}$$

$$P(x_0, t_0 | x_2 t_2) = \int P(x_0 t_0 | x_1 t_1)\, dx_1\, P(x_1 t_1 | x_2 t_2)$$

↗ Markovian stochastic process

$$\frac{\partial P(x,t)}{\partial t} - D\frac{\partial^2 P(x,t)}{\partial x^2} = \delta(t-t_0)\,\delta(x-x_0)$$

$$P(x,t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \tilde{P}(k,\omega)\, e^{i(\omega t - kx)}\, dk\, d\omega$$

$$\iint \tilde{P}(k,\omega)\left[(i\omega) - D(-ik)^2\right] e^{i(\omega t - kx)}\, dk\, d\omega = \frac{1}{(2\pi)^2}\iint \underbrace{1}_{e^{-i(\omega t_0 - kx_0)}}\, e^{i(\omega t - kx)}\, dk\, d\omega$$

$$\tilde{P}(k,\omega) = \frac{1}{(2\pi)^2}\frac{e^{-i(\omega t_0 - kx_0)}}{-Dk^2 + i\omega}$$

$$P(x,t) = \int_{-\infty}^{\infty} dk \int_{-\infty}^{\infty} d\omega \frac{1}{(2\pi)^2} \frac{e^{i[\omega(t-t_0) \mp k(x-x_0)]}}{-Dk^2+i\omega} = ?$$

$$\frac{\partial}{\partial t}\left\{\frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}\right\} = \frac{1}{\sqrt{4\pi D}} \frac{\left(-\frac{1}{2}\right)}{t^{3/2}} e^{-\frac{x^2}{4Dt}} + \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}} \left[\frac{x^2}{4Dt^2}\right]$$

$$= \frac{1}{\sqrt{4\pi D t}}\left[-\frac{1}{2t} + \frac{x^2}{4Dt^2}\right] e^{-\frac{x^2}{4Dt}}$$

$$\frac{\partial}{\partial x}\left\{\frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}\right\} = \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi D t}}\left[-2\frac{x}{4Dt}\right]$$

$$\frac{\partial^2}{\partial x^2}\{\quad\} = \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi D t}}\left[\frac{x^2}{4D^2t^2} - \frac{1}{2Dt}\right] = \frac{\partial}{\partial t}\{\quad\}\cdot\frac{1}{D}$$

$$D^2\frac{\partial^2}{\partial x^2}P \qquad \int_{-\infty}^{\infty} P(x,t)\,dx = 1$$

$$P(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}} \qquad \text{set } x_0 = t_0 = 0$$

prob. that partile is at locatio x at time t, $\langle x(t)\rangle = 0$

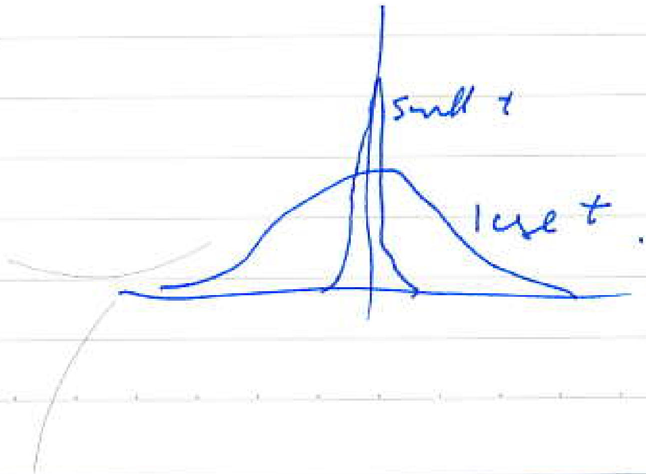
$$\langle x(t)^2\rangle = \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}} x^2\,dx \qquad \frac{x^2}{2Dt} = y^2$$

$$x = \sqrt{2Dt}\,y$$

$$= \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi D t}} e^{-\frac{y^2}{2}}\, 2Dt\, y^2 \sqrt{2Dt}\,dy$$

$$= 2Dt \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} y^2 e^{-\frac{y^2}{2}} dy = 2Dt$$

mean square dispacemnt $= 2Dt$



A Brownian particle can be modeled as random walk

$$x(t) = \sum_{i=1,2,\dots t/\Delta t} \xi_i \, a$$

each step move to left or right with equal probability by a in time Δt.

$$\langle x(t) \rangle = 0 \qquad \langle \xi_i \rangle = 0$$

total # of $N = \frac{t}{\Delta t}$

ξ_i random value with prob $+\frac{1}{2}$ $+1$, $+\frac{1}{2}$ -1

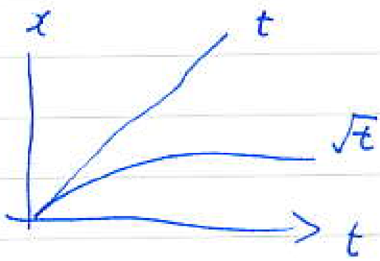
$$\langle \xi_i \xi_j \rangle = \delta_{ij}$$

$$\langle x(t)^2 \rangle = \sum_{i=1}^{N} \sum_{j=1}^{N} \langle \xi_i \xi_j \rangle a^2 = N a^2 = t \frac{a^2}{\Delta t} = 2Dt$$

we can identify $D = \frac{1}{2} \frac{a^2}{\Delta t}$ $\qquad [D] = L^2 T^{-1}$ $\quad m^2 sec^{-1}$

ballistic motion $x \sim vt$

diffusive motion $x \sim \sqrt{Dt}$



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from diffusion equation to $\langle x^2 \rangle = 2Dt$

$$\frac{\partial n}{\partial t} = D \frac{\partial^2 n}{\partial x^2}$$ $n \to$ density of particle or prob of a single particle

n is treated as probability $\int n \, dx = 1$

$\langle x^2 \rangle = \int_{-\infty}^{+\infty} x^2 n(x) \, dx$ average on ensemble points

$$x^2 \frac{\partial n}{\partial t} = D x^2 \frac{\partial^2 n}{\partial x^2}$$

$n(\pm\infty) = 0$

integrate: $$\frac{\partial \langle x^2 \rangle}{\partial t} = D \int dx \, x^2 \frac{\partial^2 n}{\partial x^2}$$

$$= D \left[x^2 \frac{\partial n}{\partial x} \Big|_{-\infty}^{+\infty} - \int \frac{\partial x^2}{\partial x} \frac{\partial n}{\partial x} dx \right]$$

$$= D \int 2x \frac{\partial n}{\partial x} dx = D \left[2x n \Big| + \int 2 n \, dx \right]$$

$$= 2D$$

$\langle x^2 \rangle = 2Dt$ assume $\langle x^2 \rangle = 0$ at $t = 0$.

Langevin Eq Date 22 March 07

and solution $\begin{cases} \langle v \rangle \\ \langle v^2 \rangle \quad \langle v(0)\, v(t) \rangle \\ \langle x^2 \rangle \end{cases}$

fluctuation dissipation theorem

work in 1D (high dimens is similar)

$\langle \ \rangle$ average over what ?

Stochastic differential Eq.

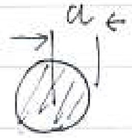
$$m\frac{dv}{dt} = \underset{\text{friction}}{-m\gamma v} + \underset{\text{random noise}}{R(t)}$$

$\langle R(t) \rangle = 0$

$\langle R(t) R(t') \rangle = C\,\delta(t-t')$

white noise

C is Not abitrary if the system is in thermal equilibrium



in fluid

$m\gamma = 6\pi a \eta$.

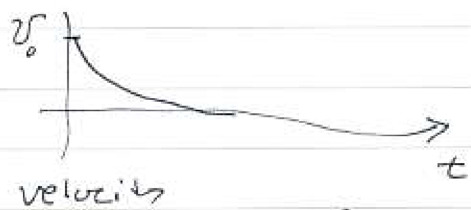
$$F = -6\pi a \eta v \quad \text{(Stokes law)}$$

η viscosity of fluid

$\langle v \rangle$

$$m\frac{d\langle v \rangle}{dt} = -m\gamma\langle v \rangle \qquad \frac{d\langle v \rangle}{dt} = -\gamma\langle v \rangle$$

$$\rightarrow \langle v \rangle = v_0 e^{-\gamma t}$$



average velocity decay to zero for any initial velocity

Let $v = A(t) e^{-\gamma t}$ ← method of variation of constant

$$\frac{dv}{dt} = \dot{A}(t) e^{-\gamma t} - \cancel{\gamma A(t) e^{-\gamma t}} = \cancel{-\gamma A(t) e^{-\gamma t}} + \frac{R(t)}{m}$$

Date

$$\dot{A}(t) = \frac{1}{m} e^{\gamma t} R(t)$$

$$A(t) = \int_0^t \frac{1}{m} e^{\gamma t'} R(t')\, dt' + A(0)$$

$$v(t) = \left[\frac{1}{m}\int_0^t e^{\gamma t'} R(t')\, dt' + A(0)\right] e^{-\gamma t}$$

$$= \frac{1}{m}\int_0^t e^{-\gamma(t-t')} R(t')\, dt' + v(0)\, e^{-\gamma t}$$

again $\langle v(t)\rangle = v(0)\, e^{-\gamma t}$ as expected $\langle R\rangle = 0$

$$\langle v(t)\, v(t')\rangle = \left\langle \frac{1}{m}\int_0^t e^{-\gamma(t-\tau)} R(\tau)\, d\tau \; \frac{1}{m}\int_0^{t'} e^{-\gamma(t'-\tau')} R(\tau')\, d\tau' \right\rangle$$

cross terms vanish because $\langle R(t)\, v_0\rangle = 0$

$$= \frac{1}{m^2}\int_0^t d\tau \int_0^{t'} d\tau'\, e^{-\gamma(t-\tau+t'-\tau')} \underbrace{\langle R(\tau)\, R(\tau')\rangle}_{C\,\delta(\tau-\tau')}$$

assuming $t' > t$

$$= \frac{1}{m^2}\int_0^t d\tau \int_0^{t'} d\tau'\, e^{-\gamma(t-\tau+t'-\tau')}\, C\, \underline{\delta(\tau-\tau')}$$

$$= \frac{C}{m^2}\int_0^t d\tau\, e^{-\gamma(t+t'-2\tau)} = \frac{C}{m^2} e^{-\gamma(t+t')}\int_0^t e^{2\gamma\tau}\, d\tau$$

$$= \frac{C}{m^2} e^{-\gamma(t+t')} \frac{1}{2\gamma}\left[e^{2\gamma t} - 1\right]$$

$$= \frac{C}{2m^2\gamma}\left[e^{-\gamma(t'-t)} - e^{-\gamma(t+t')}\right]$$

$$\simeq \frac{C}{2m^2\gamma} e^{-\gamma(t'-t)}$$

t, t' large

$|t-t'|$ small

in genl $\langle v(t)\, v(t') \rangle = \frac{C}{2m^2\gamma} e^{-\gamma|t'-t|}$

Date

Einstein :

$$\frac{1}{2} m \langle v^2 \rangle = \frac{1}{2} k_B T$$

$$\langle v^2 \rangle = \frac{k_B T}{m} = \langle v(t)\, v(t) \rangle = \frac{C}{2m^2\gamma}$$

$$\rightarrow \quad C = 2m\gamma k_B T$$

$$\langle R(t)\, R(t') \rangle = 2m\gamma k_B T\, \delta(t-t') \rightarrow$$

fluctuation dissipation theorem

random force must be related to the friction to reach equilibrium

mean-square displacement

$\langle x^2(t) \rangle$

$$x(t) = \int_0^t v(\tau)\, d\tau \qquad \text{assume } x(0) = 0$$

$$\langle x(t)^2 \rangle = \langle \int_0^t v(\tau) d\tau \int_0^t v(\tau') d\tau' \rangle$$

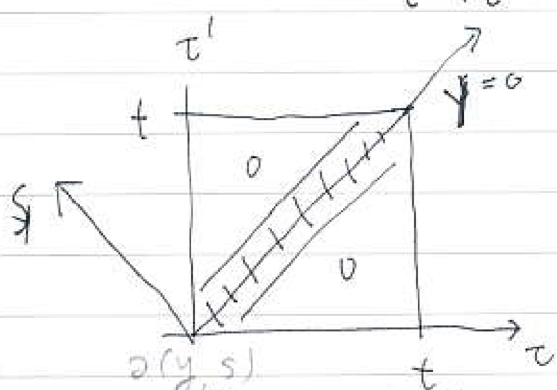
translational invariance

$$= \int_0^t d\tau \int_0^t d\tau' \langle v(\tau)\, v(\tau') \rangle = \int_0^t d\tau \int_0^t d\tau' \langle v(0)\, v(\tau'-\tau) \rangle$$

$$= \int_0^t d\tau \int_{-\tau}^{t-\tau} ds \langle v(0)\, v(s) \rangle$$

$\tau' - \tau = s$

$\tau' + \tau = y$



$$= \int dy\, ds\, \frac{\partial(\tau,\tau')}{\partial(y,s)} \langle v(0)\, v(s) \rangle$$

$$= \frac{1}{2} \int_0^{2t} dy \int_{-\infty}^{\infty} ds \langle v(0)\, v(s) \rangle$$

$$\frac{\partial(s,y)}{\partial(\tau,\tau')} = \begin{vmatrix} \frac{1}{2} & +\frac{1}{2} \\ +\frac{1}{2} & +\frac{1}{2} \end{vmatrix} = +\frac{1}{2}$$

$$= t \int_{-\infty}^{\infty} ds \langle v(0)\, v(s) \rangle$$

$$\langle x(t)^2 \rangle \underset{t \text{ large}}{\approx} 2t \int_0^\infty \langle v(0)\, v(s) \rangle\, ds = \cancel{2tD} = 2Dt$$

Date

$$\rightarrow \quad \underbrace{D}_{\text{Diffusion constant}} = \underbrace{\int_0^\infty \langle v(0)\, v(s) \rangle\, ds}_{\text{Green-Kubo formula}} = \int_0^\infty \frac{k_B T}{m} e^{-\gamma s}\, ds$$

$$= \frac{k_B T}{m\gamma} = \frac{k_B T}{6\pi \eta a}$$

Einstein's relation

How to compute $\langle v(t_1)\, v(t_2) \cdots v(t_n) \rangle$?

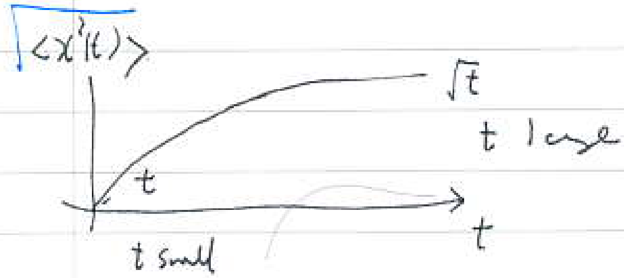
Need assumptions about high-order correlations of R

the simplist is gaussian process

$$\underbrace{\langle R(t_1) \cdots R(t_n) \rangle}_{\text{if } n \text{ is odd}} = 0$$

$$\langle R(t_1) \cdots R(t_n) \rangle = \sum_{\text{all possible pairing}} \langle \quad \rangle \langle \cdots \rangle$$

(c.f. Wick theorem)



Green-Kubo-type formulae for transport coeffict

self-diffusion constant $\quad D = \int_0^\infty \langle v(0)\, v(t) \rangle_{eq}\, dt \qquad j = -D \nabla n$

Thermal ~~const~~ conductivity $\quad \kappa = \cdots \int \langle j(0)\, j(t) \rangle_{eq}\, dt \qquad \vec{q} = -\kappa \nabla T$ (heat current)

electric $\quad \sigma \qquad \vec{j} = \sigma \vec{E}$

transport coeffiants in nonequilibrium situati (but near equilibm (linear response regim) is related to equilibm correlation functions.

27 March 07

A more careful derivation

(Uhlenbeck, Ornstein process)

$$\frac{dv}{dt} = -\gamma v + \frac{R(t)}{m}$$

$$\frac{dv}{dt} = -\gamma v \rightarrow \quad v(t) = Ae^{-\gamma t}$$

$$v'(t) = \cancel{A(t)e^{-\gamma t}(-\gamma)} + A'(t)e^{-\gamma t} = \cancel{-\gamma A e^{-\gamma t}} + \frac{R(t)}{m}$$

$$A'(t) = \frac{R(t)}{m} e^{\gamma t}$$

$$A(t) = A(0) + \int_0^t \frac{R(\tau)}{m} e^{\gamma \tau} d\tau$$

$$v(t) = \left[v(0) + \int_0^t \frac{R(\tau)}{m} e^{\gamma \tau} d\tau \right] e^{-\gamma t}$$

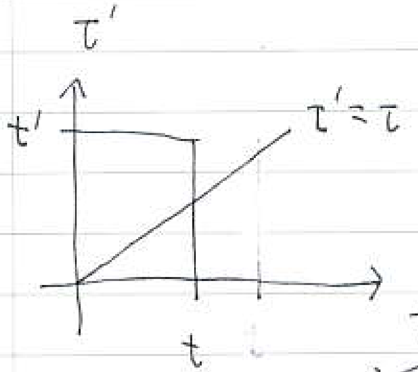
$$= v(0) e^{-\gamma t} + \int_0^t \frac{R(\tau)}{m} e^{-\gamma(t-\tau)} d\tau$$

assume initial velocity is indep. of R: $\langle v(0) R(\tau) \rangle = 0$

$$\langle v(t) v(t') \rangle = v(0)^2 e^{-\gamma(t+t')}$$

$$+ \int_0^t d\tau \frac{e^{-\gamma(t-\tau)}}{m} \int_0^{t'} d\tau' \frac{e^{-\gamma(t'-\tau')}}{m} \langle R(\tau) R(\tau') \rangle$$

$$= v^2(0) e^{-\gamma(t+t')} + \int_0^t d\tau \frac{e^{-\gamma(t-\tau)}}{m} \int_0^{t'} d\tau' \frac{e^{-\gamma(t'-\tau')}}{m} C\,\delta(\tau-\tau')$$



let assume $t' > t$

$$= v^2(0) e^{-\gamma(t+t')} + \int_0^t d\tau \frac{C e^{-\gamma(t-\tau)}}{m^2} e^{-\gamma(t'-\tau)}$$

$$= v^2(0) e^{-\gamma(t+t')} \cancel{+ \frac{1}{m^2} e^{-\gamma(t'-2\tau)} \int_0^t e^{-\gamma t} d}$$

$$= v(0)e^{-\gamma(t+t')} + \frac{C}{m^2} e^{-\gamma(t+t')} \int_0^t e^{2\gamma\tau} d\tau$$

$$= v(0) e^{-\gamma(t+t')} + \frac{C}{m^2} e^{-\gamma(t+t')} \left[\frac{1}{2\gamma}\left(e^{2\gamma t} - 1\right)\right]$$

$$= v^2(0) e^{-\gamma(t+t')} + \frac{C}{2\gamma m^2}\left[e^{-\gamma(t'-t)} - e^{-\gamma(t+t')}\right] \qquad t' > t$$

In a stationary process t, t' large large $t - t'$ small

$$x(t) = \int_0^t v(t')\,dt' \qquad x(t=0) = 0 \qquad t'' - t' = s$$

$$\langle x^2(t)\rangle = \left\langle \int_0^t v(t')\,dt' \int_0^t v(t'')\,dt'' \right\rangle = \int_0^t dt' \int_0^t dt'' \langle v(t')v(t'')\rangle$$

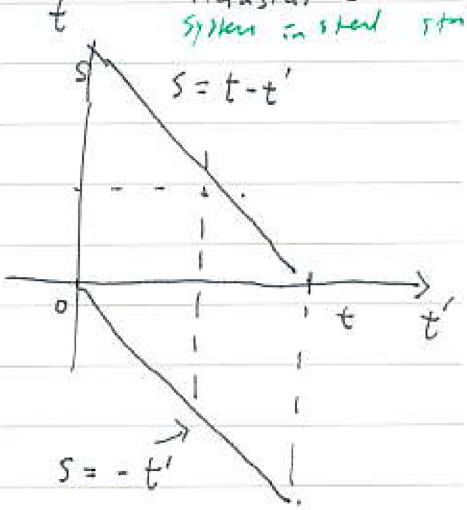
$$= \langle v(0)v(t''-t')\rangle$$

translational invariance

system in steady state

$$= \int_0^t dt' \int_0^t dt'' \langle v(0)v(s)\rangle \Big|_{s = t''-t'}$$

$$s = t'' - t'$$



$$= \int_0^t dt' \int_{-t'}^{t-t'} ds \langle v(0)v(s)\rangle$$

$$= \int_0^t ds \int_0^{\cancel{t}-s} dt' \langle v(0)v(s)\rangle + \int_{-t}^{0} ds \int_{-s}^{t} dt' \langle v(0)v(s)\rangle$$

$$\langle v(0)v(s)\rangle = \langle v(0)v(-s)\rangle$$

$$= \int_0^t ds\, (t-s)\langle v(0)v(s)\rangle + \int_{-t}^0 ds\,(t+s)\langle v(0)v(s)\rangle$$

$$s \to -s$$

$$= 2\int_0^t ds\,(t-s)\langle v(0)v(s)\rangle$$

$t \to \infty$ $\langle v(0)v(s)\rangle$ short-ranged. $\langle x^2(t)\rangle = 2t \int_0^t \langle v(0)v(s)\rangle$

$$= 2tD$$

using $\langle v(0)\, v(s) \rangle = \frac{C}{2m^2\gamma} e^{-\gamma|s|} = \frac{k_BT}{m} e^{-\gamma|s|}$

Date

$$\langle x^2(t) \rangle = 2\int_0^t ds\, (t-s) \frac{k_BT}{m} e^{-\gamma s}$$

$$= \frac{2k_BT}{m}\left[t\int_0^t ds\, e^{-\gamma s} - \int_0^t s e^{-\gamma s} ds \right]$$

$$= \frac{2k_BT}{m}\left[\frac{-t}{\gamma}\left(e^{-\gamma t}-1\right) - \frac{(-1)}{\gamma}\int_0^t s\, d e^{-\gamma s} \right]$$

$$= \frac{2k_BT}{m\gamma}\left[\left(1-e^{-\gamma t}\right)t + \cancel{\frac{\gamma}{\gamma}}\, s e^{-\gamma s}\Big|_0^t - \int_0^t e^{-\gamma s} ds \right]$$

$$= \frac{2k_BT}{m\gamma}\left[t - \cancel{e^{-\gamma t} t} + \cancel{t e^{-\gamma t}} + \frac{1}{\gamma}\left(e^{-\gamma t}-1\right) \right]$$

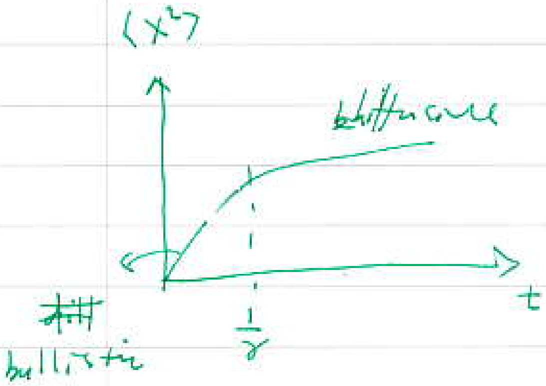
$$= \frac{2k_BT}{m\gamma}\left(t - \frac{1}{\gamma}\left(1-e^{-\gamma t}\right) \right)$$

$$= \begin{cases} \frac{2k_BT}{m\gamma}\, t & t\to\infty \\ \frac{k_BT}{m}\, t^2 & t \to 0 \\ \langle v^2 \rangle t^2 & \end{cases}$$

$D = \frac{k_BT}{m\gamma}$

$\cancel{t} - \frac{1}{\gamma}\left(\cancel{1} + \gamma \cancel{t} \mp \frac{1}{2}(\gamma t)^2\right)$

$+ \frac{1}{2}\gamma t^2$



$D = \frac{k_BT}{m\gamma} = \frac{k_BT}{6\pi a \eta}$

a: size of the molecule

η: viscosity

Fourier Analysis $\qquad z(t)$ is real

Let $z(t)$ periodic function in $0 \le t \le T$ $\quad (T_{\text{Data}} \to \infty)$

Fourier series
$$z(t) = \sum_{n=-\infty}^{\infty} a_n e^{i\omega_n t} \qquad \omega_n = \frac{2\pi n}{T} \qquad n = 0, \pm 1, \pm 2, \ldots$$
a_n: complex number

$$a_n = \frac{1}{T}\int_0^T z(t)\, e^{-i\omega_n t}\, dt$$

go ver to Fourier integral by $T \to \infty$, $\Delta\omega = \frac{2\pi}{T}$

$$z(t) = \int_{-\infty}^{\infty} a(\omega)\, e^{-i\omega t}\, \frac{d\omega}{2\pi} \qquad a_n \to a_n \frac{2\pi}{T} \ (\omega)$$

change convention of Fourier transform

$$a(\omega) = \int_{-\infty}^{\infty} z(t)\, e^{+i\omega t}\, dt$$

since $z(t)$ is real $\quad a^*(\omega) = a(-\omega)$

Wiener - Khintchine theorem:

power spectrum in ω-space is correlation in time space

correlation function $\qquad$ assume ① $\langle z(t) \rangle \equiv 0$

$$\phi(t) = \langle z(t_0)\, z(t_0 + t) \rangle$$
② translational invariant

consider ~~$I(\omega) =$~~

$$I(\omega) = \int_{-\infty}^{\infty} \phi(t)\, e^{+i\omega t}\, dt \qquad z(t') = \int_{-\infty}^{\infty} a(\omega)\, e^{i\omega t'}\, d\omega$$

$$= \int_{-\infty}^{\infty} dt\, e^{+i\omega t} \langle z(t_0)\, z(t_0 + t) \rangle$$

$$= \int_{-\infty}^{\infty} dt\, e^{+i\omega t} \left\langle \int_{-\infty}^{\infty} a(\omega')\, e^{-i\omega' t_0}\, \frac{d\omega'}{2\pi} \int_{-\infty}^{\infty} a(\omega'')\, e^{-i\omega''(t_0 + t)}\, \frac{d\omega''}{2\pi} \right\rangle$$

z is real

$$\langle a(\omega)\,\overset{*}{a}(\omega')\rangle = \Big\langle \cancel{\tfrac{1}{2\pi}}\int_{-\infty}^{\infty} z(t)\, e^{+i\omega t}\, dt\ \cancel{\tfrac{1}{2\pi}}\int_{-\infty}^{\infty} z(t')\, e^{-i\omega' t'}\, dt' \Big\rangle$$

Date

$$= \boxed{\cancel{\tfrac{1}{(2\pi)^2}}}\int dt \int dt' \underbrace{\langle z(t)\, z(t')\rangle}_{\cancel{\phi(t'-t)}\ \phi(t-t')} e^{-i(\omega' t' - \omega t)}$$

Let ~~$t'-t = t''$~~ $t - t' = t''$

$$= \boxed{\cancel{\tfrac{1}{(2\pi)^2}}}\int dt \int dt''\, \phi(t'')\, e^{i(\omega' t'' + \omega' t - \omega t)}$$

$$= \boxed{\cancel{\tfrac{1}{2\pi}}}\int_{-\infty}^{\infty} \phi(t'')\, e^{+i\omega' t''}\ \boxed{\cancel{\tfrac{1}{2\pi}}}\int_{-\infty}^{\infty} dt\, e^{-i(\omega'-\omega)t}$$

$$= I(\omega')\,\delta(\omega'-\omega)\cdot 2\pi \quad \Leftarrow \text{ different } \omega \text{ are uncorrelated!}$$

$$= I(\omega)\,\delta(\omega-\omega')\cdot 2\pi$$

$\rightarrow \langle |a(\omega)|^2\rangle = I(\omega)\frac{T}{2\pi}$, $T \to \infty$

white noise $\langle R(t)\, R(t')\rangle = C\,\delta(t-t')$

Let $\tilde{R}[\omega] = \cancel{\tfrac{1}{2\pi}}\int_{-\infty}^{\infty} R(t)\, e^{+i\omega t}\, dt$

using above result.

$$\langle \tilde{R}[\omega]\, \tilde{R}^*[\omega']\rangle = I_R[\omega]\,\delta(\omega-\omega')\cdot 2\pi$$

power spectrum of $\delta(t-t')$ correlated noise in ω-space is

$$I_R[\omega] = \boxed{\cancel{\tfrac{1}{2\pi}}}\int_{-\infty}^{\infty} C\,\delta(t)\, e^{+i\omega t}\, dt = \frac{C}{\boxed{\cancel{2\pi}}} \quad \text{indpt of } \omega.$$

Is the Langevin Eq still valid if $\tilde{R}$ is not white noise? $\longrightarrow$ NO

Colored noise

"Generalized Langevin Eq. gives colored noise"

$$\frac{dV}{dt} = -\int_{-\infty}^{t} \gamma(t-t')V(t')\,dt' + \frac{R(t)}{m}$$

memory effect

fluctuation-Dissipation means

$\langle R(t) R(t') \rangle = mkT\gamma(t-t')$

$$V(t) = \int_{-\infty}^{\infty} \tilde{v}[\omega] e^{-i\omega t} \frac{d\omega}{2\pi} \qquad R(t) = \int_{-\infty}^{\infty} \tilde{R}[\omega] e^{-i\omega t} \frac{d\omega}{2\pi}$$

similarly for $\tilde{\gamma}[\omega]$

$$\int_{-\infty}^{\infty} \tilde{v}[\omega][-i\omega] e^{-i\omega t} \frac{d\omega}{2\pi} = -\int_{-\infty}^{t} \gamma(t-t') \int_{-\infty}^{\infty} \tilde{v}[\omega] e^{-i\omega t'} \frac{d\omega}{2\pi} dt' = \frac{\int \tilde{R}[\omega] e^{-i\omega t} \frac{d\omega}{2\pi}}{m}$$

$$= -\int_{-\infty}^{t} \gamma(\underline{t-t'}) e^{i\omega t'} dt' \; \tilde{v}[\omega]\,d\omega =$$

$$t-t' = t'' \qquad t' = t-t''$$

$$= -\int_{+\infty}^{0} d(-t'') e^{i\omega(t-t'')} \underset{\gamma(t'')}{} \tilde{v}[\omega]\,d\omega$$

$$= \int_{-\infty}^{\infty} d\omega\, \tilde{v}[\omega] \left(-\int_{0}^{\infty} \gamma(t'') e^{-i\omega t''} dt'' \right) e^{i\omega t}$$

remember $\gamma(t) = \begin{cases} \gamma(t) & t \geq 0 \\ 0 & t < 0 \end{cases}$

define $\gamma(t) = 0$ if $t < 0$

$$= \int_{-\infty}^{\infty} d\omega \left[-\tilde{v}[\omega] \tilde{\gamma}[\omega] \right] e^{i\omega t}$$

$$\rightarrow \quad \tilde{v}[\omega](-i\omega) = -\tilde{v}[\omega]\tilde{\gamma}[\omega] + \frac{\tilde{R}[\omega]}{m}$$

$$\rightarrow \quad \tilde{v}[\omega] = \frac{\tilde{R}[\omega]/m}{-i\omega + \tilde{\gamma}[\omega]}$$

$$I_v[\omega] = \int \langle v(0)\, v(t)\rangle e^{+i\omega t}\, dt$$

$$I_v[\omega] = \frac{1}{m^2} \frac{I_R[\omega]}{|-i\omega + \tilde{\gamma}[\omega]|^2}$$ by Wiener-Khintchine theorem

$I_R[\omega] = m k T \tilde{\gamma}[\omega] \cdot 2$

Fourier transf. of $\gamma(t)$ not the same as that in damping kernel!

problem of sedimentation / charged particle in a field

discuss this when presenting $D = \frac{k_B T}{6\pi\eta a}$

$$m\frac{dv}{dt} = -m\gamma v + f + R(t)$$

mobility

$$-m\gamma\langle v\rangle + f = 0 \qquad \langle v\rangle = \frac{1}{m\gamma} f = \mu f$$

$$\mu = \frac{1}{m\gamma}$$

$$D = \frac{k_B T}{m\gamma} \quad \text{so} \quad \frac{D}{\mu} = k_B T \leftarrow \text{"Einstein relation"}$$

Gauss distribution $\ln \Phi(\lambda) = \langle x\rangle_c + \frac{1}{2}\lambda^2 \langle x^2\rangle_c$

$\lambda \to i\xi$

How to solve the stochastic differential equation numerically?

moment generating function

$$\Phi(\lambda) = \langle e^{\lambda x}\rangle = \sum \frac{\lambda^n}{n!}\langle x^n\rangle$$

cumulant

$$\ln \Phi(\lambda) = \sum_n \frac{\lambda^n}{n!}\langle x^n\rangle_c$$

$\langle x\rangle_c = \langle x\rangle$

$\langle x^2\rangle_c = \langle x^2\rangle - \langle x\rangle^2$

$$m\frac{dv}{dt} = F + R(t)$$

$$\rightarrow m\, dv = F dt + R(t)\, dt$$

$$m\big(v(t+h) - v(t)\big) = Fh + \int_0^h R(t)\, dt$$

$$= F\cdot h + \xi$$

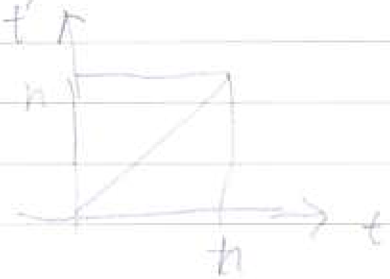
$$x = \xi = \int_0^h R(t)\, dt, \qquad \langle \xi\rangle = \int_0^h \langle R(t)\rangle dt = 0$$

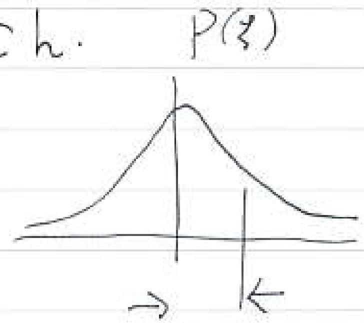
$$\langle \xi^2\rangle = \left\langle \int_0^h R(t)dt \int_0^h R(t')dt'\right\rangle = \int_0^h dt \int_0^h dt' \langle R(t) R(t')\rangle$$

$$\langle \xi^2 \rangle = \int_0^h dt \int_0^h dt' \, C \, \delta(t-t') = Ch$$

at each time-step h, generate a gaussian random number

ξ with mean zero, variance Ch.





$\sqrt{Ch}$

standard deviation

strong damping case (Smoluchowsik ?)

$$m \frac{dv}{dt} = -Kv + R(t) \qquad m = 0$$

K large

$$v = \frac{R(t)}{K} = \frac{dx}{dt}$$

$$x(t) = \frac{1}{K} \int_0^t R(t') dt'$$

$$\langle x(t) x(t') \rangle = \frac{1}{K^2} \langle \int_0^t R(t_1) dt_1 \int^{t'} R(t_2) dt_2 \rangle$$

$$= \frac{1}{K^2} \int dt_1 \int dt_2 \, C \, \delta(t_1 - t_2) = \frac{C}{K^2} \min(t, t')$$

if $t = t'$ $\quad \langle x(t)^2 \rangle = \frac{C}{K^2} t = \frac{2m\gamma k_B T}{(m\gamma)^2} t$

Gaussian process $\quad = 2 \left(\frac{k_B T}{m\gamma} \right) t$

$$\int_{t_1}^{t_2} R(t) dt = W$$: W is a rand gausi variable with zero mean and variance $t_2 - t_1$

$C = 2m\gamma k_B T$

~~$2\pi m k_B T$~~

$$= 2 \frac{k_B T}{K} t$$