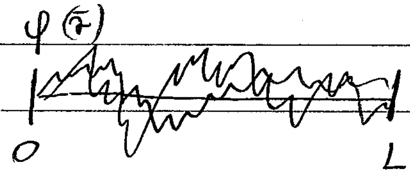
$$e^{-\beta L[\varphi(\vec r)]} = \sum_{\{S_i\}} \delta\left(\varphi(\vec r) - \frac{1}{N_\alpha}\sum_{i\in I_\alpha} S_i\right) e^{-\beta \mathcal{H}[\{S_i\}]}$$

L is a "constrained" free energy when the order parameter profile is constrained to $\varphi(\vec r)$



$$Z = \sum_{\{\varphi(\vec r)\}} e^{-\beta L[\{\varphi(\vec r)\}]}$$

↑ integration over all possible order parameter profiles (functional integral)

$$\Longrightarrow \quad Z = \int \mathcal{D}\varphi(\vec r)\, e^{-\beta L[\{\varphi(\vec r)\}]}$$

$$L = \int d^d r\, \mathcal{L}(\{\varphi(\vec r)\}) \quad , \quad \mathcal{L} = \frac{\gamma}{2}(\nabla\varphi)^2 + \frac{a t}{2}\varphi^2(\vec r) + \frac{b}{4}\varphi^4(\vec r) - h(\vec r)\varphi(\vec r)$$

$a > 0$
$b > 0$
$\gamma > 0$

evaluation, e.g., by direct discretization:

$$\int \mathcal{D}\varphi = \int \prod_{i=1}^{N} d\varphi_i$$

$$\langle \varphi(\vec r)\rangle = \frac{1}{Z}\int \mathcal{D}\varphi\; \varphi(\vec r)\, e^{-\beta L} = \frac{1}{\beta}\frac{1}{Z}\frac{\delta Z}{\delta h(\vec r)}$$

$$\langle \varphi(\vec r)\varphi(\vec r\,')\rangle = \frac{1}{Z}\int \mathcal{D}\varphi\; \varphi(\vec r)\varphi(\vec r\,')\, e^{-\beta L} = \frac{1}{\beta^2}\frac{1}{Z}\frac{\delta^2 Z}{\delta h(\vec r)\,\delta h(\vec r\,')}$$

↑

thermodynamic averages $\langle \dots \rangle$

Functional derivatives

$G[\{f(\vec{r})\}]$ $\qquad$ (e.g. $G = \int d^d r \, f^2(\vec{r})$)

$$\frac{\delta G}{\delta f(\vec{r}')} \equiv \lim_{\varepsilon \to 0} \frac{G[f(\vec{r}) + \varepsilon \delta(\vec{r} - \vec{r}')] - G[f(\vec{r})]}{\varepsilon}$$

example: (1) $G[f(\vec{r})] = \int d^d r \, f^n(\vec{r})$

$$\frac{\delta G}{\delta f(\vec{r}')} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\int d^d r \left(f(\vec{r}) + \varepsilon \delta(\vec{r} - \vec{r}') \right)^n - \int d^d r \, f(\vec{r}) \right]$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\int d^d r \left(f^n(\vec{r}) + n f^{n-1}(\vec{r}) \, \varepsilon \delta(\vec{r} - \vec{r}') + o(\varepsilon^2) \right) - \int d^d r \, f(\vec{r}) \right]$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left[\varepsilon n f^{n-1}(\vec{r}') + o(\varepsilon^2) \right] = \boxed{n f^{n-1}(\vec{r}')}$$

(2) $G[f(\vec{r})] = f(\vec{r})$

$$\boxed{\frac{\delta G}{\delta f(\vec{r}')} = \delta(\vec{r} - \vec{r}')}$$

(3) $G[f(\vec{r})] = \int d^d r \, (\vec{\nabla} f)^2$

$$\boxed{\frac{\delta G}{\delta f(\vec{r}')} = -2 \nabla'^2 f(\vec{r}')}$$ see HW

$$Z = \int \mathcal{D}\varphi \, e^{-\beta \int d^d r \, [\frac{\gamma}{2}(\nabla\varphi)^2 + \frac{a}{2} t \varphi^2 + \frac{b}{4}\varphi^4 - h(\vec r)\varphi(\vec r)]}$$

$$\chi(\vec r, \vec r\,') = \frac{\delta \langle \varphi(\vec r)\rangle}{\delta h(\vec r\,')} = \frac{\delta}{\delta h(\vec r\,')}\left\{\frac{1}{Z}\frac{\delta Z}{\beta \delta h(\vec r)}\right\}$$

$$= \frac{1}{\beta}\left\{\frac{1}{Z}\frac{\delta^2 Z}{\delta h(\vec r\,')\delta h(\vec r)} - \frac{1}{Z^2}\frac{\delta Z}{\delta h(\vec r\,')}\frac{\delta Z}{\delta h(\vec r)}\right\} =$$

$$= \beta \{ \underbrace{\langle \varphi(\vec r)\varphi(\vec r\,')\rangle - \langle \varphi(\vec r)\rangle\langle\varphi(\vec r\,')\rangle}_{G(\vec r, \vec r\,')} \}$$

$$\chi_{ij} = \frac{\partial \langle s_i \rangle}{\partial h_j} = \beta(\langle s_i s_j\rangle - \langle s_i\rangle\langle s_j\rangle)$$

$$\chi(\vec r, \vec r\,') = \frac{1}{k_B T} G(\vec r, \vec r\,') \qquad \left(= \frac{1}{k_B T} G(\vec r - \vec r\,')\right)$$

$$\chi_T = \frac{1}{k_B T}\int d^d r \, G(\vec r) \qquad \text{susceptibility sum rule}$$

Landau theory:

$$Z = \int \mathcal{D}\varphi \, e^{-\beta L[\varphi(\vec r)]} \approx e^{-\beta L_{min}} = e^{-\beta L[\bar\varphi]}$$

(i.e., considers only configuration with max. probability)

$\langle \varphi(\vec r)\rangle \simeq \bar\varphi(\vec r)$ (technically: steepest descent.)

$$L[\varphi] = \int d^d r \left\{\frac{\gamma}{2}(\nabla\varphi)^2 + \frac{a t}{2}\varphi^2 + \frac{b}{4}\varphi^4 - h(\vec r)\varphi(\vec r)\right\}$$

$$\frac{\delta L}{\delta \varphi(\vec r)} = -\gamma \nabla^2\varphi + a t\varphi + b\varphi^3 - h(\vec r) = 0$$

$\varphi \equiv \langle \varphi(\vec r)\rangle$ $\quad h(\vec r) \equiv H = 0 \qquad a t \varphi + b\varphi^3 = 0 \Rightarrow \langle\varphi\rangle \simeq \begin{cases} 0 & t > 0 \\ \sqrt{\frac{a|t|}{b}} & t < 0 \end{cases} \to \boxed{\beta = 1/2}$

$$\frac{\delta}{\delta h(\vec r\,')}: \quad -\gamma\nabla^2 \frac{\delta\varphi(\vec r)}{\delta h(\vec r\,')} + a t \frac{\delta \varphi(\vec r)}{\delta h(\vec r\,')} + 3b\varphi^2 \frac{\delta\varphi(\vec r)}{\delta h(\vec r\,')} - \delta(\vec r, \vec r\,') = 0$$

$$[-\gamma\nabla^2 + a t + 3b\varphi^2]\,\chi(\vec r, \vec r\,') = \delta(\vec r - \vec r\,')$$

$$\boxed{[-\gamma\nabla^2 + a t + 3b\varphi^2]\, G(\vec r, \vec r\,') = k_B T\, \delta(\vec r - \vec r\,')}$$

$$\left[-\nabla^2 + \frac{a}{\gamma}t + \frac{3b}{\gamma}\varphi^2\right] G(\bar{r}-\bar{r}') = \frac{k_B T}{\gamma}\delta(\bar{r}-\bar{r}')$$

the φ^2 term should be carefully treated separately for $T>T_c$ and $T<T_c$:

$$\varphi^2 = \begin{cases} 0 & T>T_c \\ \frac{-at}{b} & T<T_c \end{cases}$$

$$\left[-\nabla^2 + \frac{a}{\gamma}t\right] G(\bar{r}) = \frac{k_B T}{\gamma}\delta(\bar{r}) \qquad T>T_c$$

$$\left[-\nabla^2 + \frac{2a|t|}{\gamma}\right] G(\bar{r}) = \frac{k_B T}{\gamma}\delta(\bar{r}) \qquad T<T_c$$

$$\boxed{\left[-\nabla^2 + \xi^{-2}\right] G(\bar{r}) = \frac{k_B T}{\gamma}\delta(\bar{r})}$$

where $\xi^{-2}(t) = \begin{cases} \frac{at}{\gamma} & t>0 \\ \frac{2a|t|}{\gamma} & t<0 \end{cases}$

i.e., $\xi(t) = \begin{cases} \sqrt{\frac{\gamma}{at}} & t>0 \\ \sqrt{\frac{\gamma}{2a|t|}} & t<0 \end{cases} \Rightarrow \boxed{\xi(t) \sim |t|^{-\nu} \quad \nu = 1/2}$

"$G(\bar{r}) = \frac{k_B T}{\gamma}\frac{\delta(\bar{r})}{-\nabla^2+\xi^{-2}}$" ?

must invert $-\nabla^2+\xi^{-2}$ operator

Fourier transform:

$$G(\bar{r}) = \frac{1}{(2\pi)^d}\int d^d k\, e^{i\bar{k}\cdot\bar{r}}\,\tilde{G}(\bar{k})$$

$$\tilde{G}(\bar{k}) = \int d^d\bar{r}\, e^{-i\bar{k}\bar{r}}\, G(\bar{r})$$

$$\delta(\bar{r}) = \frac{1}{(2\pi)^d}\int d^d k\, e^{i\bar{k}\cdot\bar{r}}$$

$$\left[k^2+\xi^{-2}\right]\tilde{G}(\bar{k}) = \frac{k_B T}{\gamma} \qquad \left(\xi \sim |t|^{-1/2}\right)$$

$$\boxed{\tilde{G}(\bar{k}) = \frac{k_B T}{\gamma}\,\frac{1}{k^2+\xi^{-2}}} \qquad \Rightarrow \chi_T = \frac{1}{k_B T}\tilde{G}(k\to 0) \sim |t|^{-1}$$

$$\boxed{\gamma = 1}$$

Breakdown of Landau theory (Ginzburg criterion)

$$a \ll \overset{\text{block size}}{\ell} < \xi \quad \text{correlation length (size of coherent domains}$$

$V_\xi = \xi^d$ correlation volume

$\langle\varphi(\bar r)\rangle = \langle\varphi\rangle$

$$E_G = \frac{\iint d^d r'\, d^d r\,\left[\langle\varphi(\bar r)\varphi(\bar r')\rangle - \langle\varphi(\bar r)\rangle\langle\varphi(\bar r')\rangle\right]}{\int d^d r\, d^d r'\,\langle\varphi(\bar r)\rangle\langle\varphi(\bar r')\rangle} = \frac{\int d^d r\, G(r)}{V_\xi\,\langle\varphi\rangle^2} =$$

$$= \frac{k_B T\,\chi_T}{\xi^d\,\langle\varphi\rangle^2} \sim \frac{|t|^{-\gamma}}{|t|^{-d\nu}\,|t|^{2\beta}} = |t|^{-\gamma-2\beta+d\nu} \longrightarrow \begin{cases} 0 & d > \frac{\gamma+2\beta}{\nu} \\ \infty & d < \frac{\gamma+2\beta}{\nu} \end{cases}$$

$$\boxed{d_c \equiv \frac{\gamma+2\beta}{\nu}} \qquad \underline{\text{upper critical dimension}}$$

Landau theory ("steepest descent: $\int D\varphi\, e^{-\beta L} \approx e^{-\beta L_{min}}$) will not work for $d < d_c$. Fluctuations are important. Their size will not become relatively small compared to the mean

Ising model: $\gamma = 1$, $\beta = 1/2$, $\nu = 1/2$ $\Rightarrow \boxed{d_c = 4}$

Table 3.1 CRITICAL EXPONENTS FOR THE ISING UNIVERSALITY CLASS

Exponent	Mean Field	Experiment	Ising ($d = 2$)	Ising ($d = 3$)
α	0 (disc.)	0.110 – 0.116	0 (log)	0.110(5)
β	1/2	0.316 – 0.327	1/8	0.325±0.0015
γ	1	1.23 – 1.25	7/4	1.2405±0.0015
δ	3	4.6 – 4.9	15	4.82(4)
ν	1/2	0.625±0.010	1	0.630(2)
η	0	0.016 – 0.06	1/4	0.032±0.003

3.7.3 How Good is Mean Field Theory?

Table 3.1 compares critical exponents calculated in mean field theory with those measured in experiment or deduced from theory for the Ising model in two and three dimensions. The table is essentially illustrative: the values given are not necessarily the most accurate known at the time of writing. In addition the experimental values are just given approximately, with a range reflecting inevitable experimental uncertainty. The values for ν and δ are not independent from the other values, obtained using **scaling laws**. The experimental values quoted are actually obtained from experiments on fluid systems.[3] Our discussion of the lattice gas model implies that these fluid systems should be in the universality class of the Ising model. Indeed, this expectation is borne out by the comparison of the experimental values and those from the three dimensional Ising model. The latter values are in some cases given with the number in brackets representing the uncertainty in the last digit quoted.[4]

The numerical values of the critical exponents calculated from mean field theory are in reasonable agreement with those given by experiment and the Ising model in three dimensions, although there are clearly systematic differences. First of all, the mean field theory exponents here do not depend on dimension, whereas it is clear that the exact critical exponents do. It is possible for mean field theory to exhibit exponents with a value dependent upon dimension. An example is the mean field theory

[3] J.V. Sengers in *Phase Transitions*, Proceedings of the Cargèse Summer School 1980 (Plenum, New York, 1982).

[4] J.C. Le Guillou and J. Zinn-Justin, *Phys. Rev. B* **21**, 3976 (1980); numerical values and details of the calculational techniques used to obtain these estimates are given by J. Zinn-Justin, *Quantum Field Theory and Critical Phenomena* (Clarendon, Oxford, 1989), Chapter 25.

Exact Solution for the one dimensional Ising Chain

$d=1$ periodic boundary conditions, general H

Transfer Matrix method

$\boxed{S_{N+1} = S_1}$

$$\mathcal{H}[\{S_i\}] = -J \sum_{\langle ij \rangle} S_i S_j - H \sum_{i=1}^{N} S_i \qquad S_i = \pm 1 \qquad \forall i = 1, 2, \dots, N$$

$$Z_N(T,H) = \sum_{S_1, S_2, \dots S_N} e^{-\beta \mathcal{H}[\{S_i\}]} = \sum_{S_1, S_2, \dots S_N} e^{K \sum_{i=1}^{N} S_i S_{i+1} + h \sum_{i=1}^{N} S_i}$$

where $K = \beta J$ $\qquad h = \beta H \qquad S_{N+1} \equiv S_1$ (p.b.c.)

$$K \sum_{i=1}^{N} S_i S_{i+1} + h \sum_{i=1}^{N} S_i = K \sum_{i=1}^{N} S_i S_{i+1} + \frac{h}{2} \sum_{i=1}^{N} (S_i + S_{i+1})$$

$$Z_N(T,H) = \sum_{S_1, S_2, \dots, S_N} e^{K \sum_{i=1}^{N} S_i S_{i+1} + \frac{h}{2} \sum_{i=1}^{N} (S_i + S_{i+1})} = \sum_{S_1, S_2, \dots, S_N} \prod_{i=1}^{N} e^{K S_i S_{i+1} + \frac{h}{2}(S_i + S_{i+1})}$$

$S, S' = \pm 1$ $$T_{SS'} \equiv e^{KSS' + \frac{h}{2}(S+S')} \qquad \hat{T} = \begin{pmatrix} T_{++} & T_{+-} \\ T_{-+} & T_{--} \end{pmatrix} = \begin{pmatrix} e^{K+h} & e^{-K} \\ e^{-K} & e^{K-h} \end{pmatrix}$$

transfer matrix

$$Z_N = \sum_{S_1, S_2, \dots S_N} \prod_{i=1}^{N} T_{S_i S_{i+1}} = \sum_{S_1, S_2, \dots, S_N} T_{S_1 S_2} T_{S_2 S_3} \dots T_{S_{N-1} S_N} T_{S_N S_1} =$$

$$= \sum_{S_1} \left(\hat{T}^N\right)_{S_1 S_1} = \mathrm{Tr}\left(\hat{T}^N\right)$$

$$\boxed{Z_N(T,H) = \mathrm{Tr}\left(\hat{T}^N\right)}$$

Trace is independent of the representation: diagonal representation

$$Tr(\hat{T}^N) = Tr\Big[\underbrace{\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}\cdots\begin{pmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{pmatrix}}_{N \text{ times}}\Big] = Tr\left\{\begin{pmatrix}\lambda_1^N & 0\\ 0 & \lambda_2^N\end{pmatrix}\right\} = \lambda_1^N + \lambda_2^N$$

$$Z_N(T,H) = \lambda_1^N + \lambda_2^N$$

eigenvalues of $\hat{T}$: λ_1, λ_2

eigenvalues of $\hat{T}^N$: λ_1^N, λ_2^N

$\Rightarrow \boxed{Tr(\hat{T}^N) = \lambda_1^N + \lambda_2^N}$

Thermodynamic limit: $N \to \infty$ $\qquad |\lambda_1| > |\lambda_2|$

$$Z_N(T,H) = \lambda_1^N\left(1 + \left(\frac{\lambda_2}{\lambda_1}\right)^N\right) \simeq \lambda_1^N \qquad \left(\frac{\lambda_2}{\lambda_1}\right)^N \to 0$$

$$F(T,H,N) = -kT \ln Z_N(T,H) = -kT \ln\left[\lambda_1^N\left(1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right)\right]$$

$$f(T,H) = \frac{F(T,H,N)}{N} = -kT\ln\lambda_1 - \frac{1}{N}kT\ln\left(1+\left(\frac{\lambda_2}{\lambda_1}\right)^N\right)$$

$$\xrightarrow[N\to\infty]{} -kT\ln\lambda_1$$

$$\boxed{\begin{aligned} Z_N(T,H) &\simeq \lambda_1^N \\ f(T,H) &= -kT\ln(\lambda_1)\end{aligned}} \qquad N\to\infty$$

determine λ_1, λ_2 eigenvalues:

$$\begin{vmatrix} e^{K+h} - \lambda & e^{-K} \\ e^{-K} & e^{K-h} - \lambda \end{vmatrix} = \left(e^{K+h} - \lambda\right)\left(e^{K-h} - \lambda\right) - e^{-2K} = 0$$

$$\lambda^2 - \lambda\, 2e^K \cosh(h) + 2\sinh(2K) = 0$$